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Abstract. Optimal experiment design is the definition of the conditions under which an experiment is to be conducted in order to maximize the accuracy with which the results are obtained. This paper summarizes a number of methods by which the parameters of the mathematical model of the system are estimated and describes the application of the Fisher information matrix. Examples are given for thermal property estimation in which the estimation is affected both by measurement noise, which is present during any experiment, but also by uncertainties in the parameters of the model used to describe the system.

Keywords: sensors, parameter estimation, inverse problems, sensitivity analysis, optimization, mathematical models, least squares approximations, random processes, experimental design, information matrix

Nomenclature

$\boldsymbol{b}$	Uncertain parameter vector
c	Specific heat capacity
$\boldsymbol{E}[\,]$	Expected value operator
f	Probability density function
Fo	Fourier number
$\mathbf{G}$	Covariance matrix of uncertain parameters
k	Thermal conductivity
K	Number of observations
$\mathbf{M}$	Fisher information matrix
m	Number of parameters to be estimated
N	Number of data points
n_{b}	Number of uncertain parameters
$\boldsymbol{P}$	Vector of known and uncertain parameters
q_x	Heat flux
$\mathbf{S}$	Covariance matrix
t	Time
T	Temperature
$\boldsymbol{u}$	Unknown parameter vector
x, y	Sensor position
$\boldsymbol{z}$	Measured data vector
ρ	Density
$\boldsymbol{\Theta}$	Vector of parameters to be estimated
σ	Standard deviation

1. Introduction

Let us consider a system whose behaviour is represented by a mathematical model, for example a partial differential equation. This mathematical model contains parameters, some of which are unknown or uncertain. What we want to do is to conduct an experiment in which we measure the system response in such a way that we can best deduce the values of these unknown parameters. We will refer to the definition of the experiment, that is the specification of the boundary conditions, initial conditions, sensor locations, etc, as the experimental protocol. Deduction of the values of the parameters of the model is called parameter estimation. We must also be concerned with observability (can the measurements be obtained given the parameters?) and identifiability (will the measurements permit us to deduce the values of the parameters? Banks and Kunisch 1989)†. Although the concepts and approaches described here are applicable to any system, for example mechanical, dynamic or economic, we will concentrate on thermal systems. The reader should have no difficulty in applying the concepts to another system. The definition of the protocol should be such that the parameters are estimated with the greatest exactness, that is, in a statistical sense the estimated values will approach the true parameter values with a minimum of error.

Let $z_{ij} = z(x_i, y_i, t_j)$ be the response measured at a location x_i, y_i and time t_j. We assume that z_{ij} is a function of the material properties k, ρ, c, the system dimensions L, the boundary conditions B, the initial conditions I, and any other relevant quantities (i.e. local heat generation). Then we model the system by

$$z_{ij} = F(x_i, y_i, t_j, k, B, \ldots, I) \tag{1}$$

where $B, \ldots, I$, may be functions of time, space, and of z itself. However, we also know that the properties of real materials are often not invariant and that there may be errors in the measurements and uncertainties in sensor locations,

† The question of identifiability will be addressed in a later section.

sampling times, boundary conditions, initial conditions and any other variables used to define the protocol and the system response. Thus we write equation (1) as

$$z_{ij} = F(\overline{x}_i, \delta x_i, \overline{y}_i, \delta y_i, \overline{t_j}, \delta t_j, \mu_k, \sigma_k^2, \mu_B, \sigma_B^2, \ldots . \mu_I, \sigma_I^2) + e_{ij} \quad (2)$$

where we have indicated impreciseness in quantities which are usually considered to be deterministic by writing them in terms of average values and deviations (e.g. $\overline{x}_i, \delta x_i$) and in those that are intrinsically random, and thus defined by a probability distribution, by expressing them in terms of their statistical characteristics (e.g. the mean μ_k and the variance σ_k^2). Depending upon the system and the experiment, quantities may be considered deterministic in some experiments and random in others.

We divide the parameters of the model into two groups as follows.

1. Those usually considered as the independent variables of the problem, e.g. sensor location and sampling times, and others normally specified, e.g. boundary conditions. These parameters will be represented by the vector $\boldsymbol{P}$. Of these, let there be n_b parameters, represented by the vector $\boldsymbol{b}$ which have some uncertainty. These will be specified in terms of their averages and deviations if they are deterministic and by their means and variances if random.

2. The parameters we seek to estimate, for example the conductivity or a boundary flux. In addition, we may also wish to estimate the variance or other statistical characteristics of these parameters. The set of all m quantities to be estimated will be referred to as parameters and denoted by the vector $\boldsymbol{\Theta}$.

The grouping of the model parameters into the sets $\boldsymbol{P}$ and $\boldsymbol{\Theta}$ is not fixed. In one experiment we may seek to estimate conductivity, in another both conductivity and specific heat capacity, in another the sensor location, and in yet another the dimensions of system. Likewise members of the set $\boldsymbol{P}$ are not immutable. At times we may wish to determine the effect of variations in boundary conditions on our estimate of conductivity, while at other times we will seek the effect of imprecision in sensor location.

From equation (2), given a deterministic system response F, the probability density distribution for z_{ij} is the probability density distribution for the error e_{ij}. Since F is a function of $\boldsymbol{\Theta}$ we write the probability density distribution for the vector of responses $\boldsymbol{z}$ as

$$f(\boldsymbol{z}) = f(\boldsymbol{z}|\boldsymbol{\Theta}) = f(e) \quad (3)$$

where we have written $f(\boldsymbol{z}|\boldsymbol{\Theta})$ to emphasize that $f(\boldsymbol{z})$ depends upon the sought after parameters $\boldsymbol{\Theta}$. Although it is usual to assume that the errors, which may differ at each sensor location and sampling time, are random with a Gaussian distribution with zero mean (i.e. no bias errors) and known variance and correlations, other error distributions have been used (Walter and Pronzato 1996). Moffat (1988) and Abernathy *et al* (1985) discuss the role of bias in experiments. $\boldsymbol{e}$ may also be interpreted as including the effects of an inadequate model, linearization of nonlinear terms, and other not easily anticipated or quantifiable deficiencies in the mathematical model. In this more general sense, the errors may be better represented by using other distributions, e.g. gamma, beta, or weibull (Schueller 1987, Eliason 1993). We will restrict ourselves to systems for which the errors $\boldsymbol{e}$ are independent of the response $\boldsymbol{z}$, and for which the parameters $\boldsymbol{\Theta}$ are constant in time. (In general constant parameters will not suffice if F is not an accurate model of the system. When F is derived from conservation equations this is not usually a problem, except when some aspects of the system, e.g. boundary conditions, chemical reactions, are inadequately modelled.) One must be careful in defining the parameters for nonlinear problems. For example if $k = k(T)$ then when T is time dependent k will vary with time and should not be considered as a parameter. However, if we define $k(T) = \alpha + \beta T$, then α and β are the parameters and it is not an onerous or too limiting restriction to require that they be constant in time. Systems for which these assumptions are not true must be treated using more general techniques (Norton 1986, Eykhoff 1974, Priestly 1987).

We first define some statistical properties which are necessary to our development of an optimal protocol†. Let x be a random variable with a probability density distribution $f(x)$. Then the expected value of $g(x)$ is $\boldsymbol{E}[g(x)] = \int g(x) f(x)\,\mathrm{d}x$ and the variance is $var[g(x)] = \int (g(x) - \boldsymbol{E}[g(x)])^2 f(x)\,\mathrm{d}x$. Consider the vector of parameters $\boldsymbol{\Theta}$ whose true values are $\boldsymbol{\Theta}^*$ and whose joint probability density distribution is expressed as $f(\boldsymbol{\Theta}|\boldsymbol{z})$ to emphasize that it depends upon the measured response $\boldsymbol{z}$. The vector of expected values of $\boldsymbol{\Theta}$ is $\boldsymbol{E}[\boldsymbol{\Theta}] = \int \boldsymbol{\Theta} f(\boldsymbol{\Theta}|\boldsymbol{z})\,\mathrm{d}\boldsymbol{\Theta}$ and the covariance matrix is $\mathbf{S}_{\boldsymbol{\Theta}}$ whose elements are $\boldsymbol{S}_{\Theta(ij)} = \int\int (\Theta_i - \boldsymbol{E}[\Theta_i])(\Theta_j - \boldsymbol{E}[\Theta_j]) f(\Theta_i|\boldsymbol{z}) f(\Theta_j|\boldsymbol{z})\,\mathrm{d}\Theta_i\,\mathrm{d}\Theta_j$.

We write the estimated parameters as $\hat{\boldsymbol{\Theta}}$ and say that an estimator is unbiased if $\boldsymbol{E}[\hat{\boldsymbol{\Theta}}] = \boldsymbol{\Theta}^*$, is asymptotically unbiased if $\boldsymbol{E}[\hat{\boldsymbol{\Theta}}] \to \boldsymbol{\Theta}^*$ as the number of data points $N \to \infty$, and is efficient if $\boldsymbol{S}_{\hat{\boldsymbol{\Theta}}}$ is a minimum. For example, if z has a Gaussian distribution with true mean μ_z and variance σ_z^2, $\overline{z} = \sum z_i/N$ is an unbiased estimator of μ_z. On the other hand, the estimator $\sum(z_i - \overline{z})^2/N$ has an expected value of $=(N-1)\,\sigma_z^2/N$, so it is not an unbiased estimator for σ_z^2. While an unbiased estimator is generally desirable, it is not always absolutely necessary. Frequently the unbiased estimator can be corrected, i.e. define the estimator to be $\sum(z_i - \overline{z})^2/(N-1)$ and its expected value is σ_z^2. Sometimes it is impossible to correct a biased estimator (Hoel 1954). Efficiency is measured relative to the maximum information available from the data and efficiencies lower than 75% can lead to serious errors in the estimated parameters (Jeffreys 1948)

The overall goal of optimal experiment design is to define the experimental protocol to permit us to estimate $\boldsymbol{\Theta}$ with the greatest statistical confidence. This is not the same as what is often referred to as the analysis of variance (ANOVA) in statistical texts (Lorenzen and Anderson 1993) or engineering uncertainty analysis (Coleman and Steele 1989, Doebelin 1995) for these analyses seek to compute the uncertainty in the measured response, $\boldsymbol{z}$ (i.e. $\mathbf{S}[\boldsymbol{z}]$)

† See Guttman *et al* (1971) or Ang and Tang (1975) for a full exposition of the statistical properties.

and to minimize it by determining what aspects of the experiment contribute to the measurement errors.

The reader can do no better than to review Fisher's trilogy (Fisher 1990) Jeffreys' application of probability and statistics to experimental data (Jeffreys 1948) and the more recent book by Hinkelmann and Kempthorne (1994) to appreciate the goals and subtleties of experiment design. Fisher notes that conclusions drawn from experiment are often criticized because of incorrect treatment of the data, the purview of the statistician, or faulty experimental protocol, the role of the experiment designer, both of which are aspects of the single area of defining the logical structure of the experiment. In contrast to the relatively simple experiments conducted when experiment design was first developed, modern sensors and data acquisition systems have given us tremendous scope in conducting experiments (Wheeler and Ganji 1996, Doebelin 1995, Holman 1984). Although the statistical treatment of data and the conduct of the experiment (e.g. the use of graeco-latin squares, randomization) are important in experiment design, they are well covered in many available references (Federer 1955, Hicks 1973, Grove and Davis 1992). Instead, we focus our attention on optimizing the experiment in terms of sensors and boundary conditions. That is we define *optimal experiment design* as answering the following questions:

1. What experiment to run (boundary conditions, heat sources)
2. What to sense (temperature and/or heat flux)
3. Where to sense (including multiple sensors)
4. When to sense (starting times and sampling increments)
5. What sensing accuracy (sensor precision)

} to minimize the variance in $\hat{\boldsymbol{\Theta}}$.

2. Parameter estimation

Since the optimal protocol clearly depends upon the method used to estimate the parameters from the data, let us summarize the most common methods of estimation.

2.1. Bayesian cost method, MAP

Define the function $C(\hat{\boldsymbol{\Theta}}, \boldsymbol{\Theta}^*)$ to be the cost of making an error in estimating the parameter. The Bayesian cost method seeks to find that value of $\hat{\boldsymbol{\Theta}}$ which will minimize the expected cost of the estimation. Using Bayes' theorem for conditional probability of $\boldsymbol{\Theta}$ given the data $\boldsymbol{z}$,

$$f(\boldsymbol{\Theta}|\boldsymbol{z}) = f(\boldsymbol{z}|\boldsymbol{\Theta}) f(\boldsymbol{\Theta}) / f(\boldsymbol{z}) \tag{4a}$$

where $f(\boldsymbol{\Theta})$ is called the *prior* distribution of $\boldsymbol{\Theta}$ and reflects our *a priori* (or subjective) knowledge about the behaviour of $\boldsymbol{\Theta}$ and where $f(\boldsymbol{z})$ is the normalizing factor given by

$$f(\boldsymbol{z}) = \int f(\boldsymbol{z}|\boldsymbol{\Theta}) f(\boldsymbol{\Theta}) \, \mathrm{d}\boldsymbol{\Theta} \tag{4b}$$

the expected cost is

$$\text{Cost} = \int C(\hat{\boldsymbol{\Theta}}, \boldsymbol{\Theta}^*) f(\hat{\boldsymbol{\Theta}}|\boldsymbol{z}) \, \mathrm{d}\hat{\boldsymbol{\Theta}}. \tag{5}$$

The best estimate, $\hat{\boldsymbol{\Theta}}_{MC}$, is found by minimizing the cost, which requires that we must specify the cost function which is a highly subjective choice and may depend upon the system being modelled (Norton 1986). In the absence of more precise information about how errors in $\hat{\boldsymbol{\Theta}}$ affect the cost, a quadratic cost function, $C(\hat{\boldsymbol{\Theta}}, \boldsymbol{\Theta}^*) = (\hat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}^*)^T Q (\hat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}^*)$ is often assumed. Then, assuming only that Q is symmetric and positive definite, $\hat{\boldsymbol{\Theta}}_{MC}$ (often referred to as a minimum mean square error estimator) is unbiased and independent of Q and is given by

$$\hat{\boldsymbol{\Theta}}_{MC}(\boldsymbol{z}) = \boldsymbol{E}[\hat{\boldsymbol{\Theta}}|\boldsymbol{z}] = \int \hat{\boldsymbol{\Theta}} f(\hat{\boldsymbol{\Theta}}|\boldsymbol{z}) \, \mathrm{d}\hat{\boldsymbol{\Theta}}. \tag{6}$$

(If the parameter is deterministic, but unknown, $\hat{\boldsymbol{\Theta}}_{MC}$ is biased, but may be asymptotically unbiased, and the bias depends upon $\boldsymbol{\Theta}$ (Sorenson 1980))

The variance of the error in estimating the parameter can be determined only for some special cases. If we linearize equation (1) about a reference value $\boldsymbol{\Theta}'$, so that we can write

$$\boldsymbol{z} - \boldsymbol{z}' + \left.\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{\Theta}}\right|_{\boldsymbol{\Theta}'} \boldsymbol{\Theta}' = \left.\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{\Theta}}\right|_{\boldsymbol{\Theta}'} \boldsymbol{\Theta} + \boldsymbol{e} \tag{7}$$

and if $\boldsymbol{\Theta}$ and $\boldsymbol{e}$ are distributed normally with variances of $\mathbf{S}_{\boldsymbol{\Theta}}$ and $\mathbf{S}_e$ respectively but are uncorrelated, then $\hat{\boldsymbol{\Theta}}_{MC}$ is unbiased, a linear function of the data, and minimizes the covariance of the error (i.e. it is efficient)

$$\begin{aligned} &\boldsymbol{E}[(\hat{\boldsymbol{\Theta}}_{MC} - \Theta^*)(\hat{\boldsymbol{\Theta}}_{MC} - \Theta^*)^{\mathrm{T}}] = \mathbf{S}[\hat{\boldsymbol{\Theta}}_{MC}] \\ &\quad = [\mathbf{S}_{\boldsymbol{\Theta}}^{-1} + (\partial \boldsymbol{F}/\partial \boldsymbol{\Theta})^{\mathrm{T}} \mathbf{S}_e^{-1} (\partial \boldsymbol{F}/\partial \boldsymbol{\Theta})]^{-1} \end{aligned} \tag{8}$$

Systems which follow equation (7) are termed *linear in the parameters*, (LP). The case of a deterministic, but unknown parameter, can be treated simply by setting $\mathbf{S}_{\boldsymbol{\Theta}}$ to infinity.

The major difficulties with using $\hat{\boldsymbol{\Theta}}_{MC}$ are the need to specify the cost function, the prior distribution $f(\boldsymbol{\Theta})$†, and performing the difficult integrations involved in equations (4b) and (6). One simplification is to require that the best estimator be one that maximizes the probability $f(\boldsymbol{\Theta}|\boldsymbol{z})$ which is called the *a posterior* probability. Hence, the Maximum-*A-Posterior* (MAP) estimator refers to the estimate which satisfies

$$\frac{\partial f(\boldsymbol{\Theta}|\boldsymbol{z})}{\partial \boldsymbol{\Theta}} = 0 \qquad \text{at } \boldsymbol{\Theta} = \hat{\boldsymbol{\Theta}}_{MAP}. \tag{9}$$

While intuitively appealing, there is no guarantee that $\hat{\boldsymbol{\Theta}}_{MAP}$ is unbiased and there is no easy way to estimate the variance of the estimation error and if $f(\boldsymbol{\Theta})$ is skewed, $\hat{\boldsymbol{\Theta}}_{MAP}$ may give very different results from $\hat{\boldsymbol{\Theta}}_{MC}$.

† Maritz and Lwin (1989) present an interesting discussion of empirical Bayesian (EB) methods in which the prior distribution of $\boldsymbol{\Theta}$ is estimated from historical data and compare the effectiveness of EB with the standard Bayesian cost method and the maximum likelihood method. Walter and Pronzato (1996), discuss the use of maximum entropy which helps to define $f(\boldsymbol{\Theta})$ without introducing extraneous information.

2.2. Maximum likelihood

Probably the most prominent non-Bayesian method (Maritz and Lwin 1989) and one which generally produces the best estimates (Hoel 1954) is the maximum likelihood principle advocated by Fisher (Fisher 1990, Edwards 1972)† which asserts that the most likely parameters (hence the name likelihood) are those that maximize the probability of obtaining the experimentally observed data $\boldsymbol{z}$. The likelihood function L is then a function of $\boldsymbol{\Theta}$ and is given by

$$L(\boldsymbol{\Theta}) = f(\boldsymbol{z}|\boldsymbol{\Theta}) = f(\boldsymbol{e}). \tag{10}$$

The choice of $f(\boldsymbol{\Theta})$, like that of the Bayesian cost function, is subjective and dependent upon the model and the purpose of the estimation. For example, the Laplacian distribution, $f(e_i) = (1/\sqrt{2}\sigma_i)\exp(-\sqrt{2}|e_i|/\sigma_i)$ leads to the least modulus method which is better than least squares in accounting for the effect of outliers. The maximum likelihood estimator, $\hat{\boldsymbol{\Theta}}_{ML}$, is defined to be the value of $\boldsymbol{\Theta}$ which maximizes L, or equivalently the logarithm of L,

$$\frac{\partial \ln L(\boldsymbol{z}|\boldsymbol{\Theta})}{\partial \boldsymbol{\Theta}} = 0 \qquad \text{at } \hat{\boldsymbol{\Theta}} = \hat{\boldsymbol{\Theta}}_{ML}. \tag{11}$$

$\hat{\boldsymbol{\Theta}}_{ML}$ has many desirable properties: for an arbitrary $f(\boldsymbol{e})$ it is consistent, asymptotically unbiased, asymptotically efficient, and it is asymptotically Gaussian with a mean of $\boldsymbol{\Theta}^*$ and a covariance error matrix of

$$\mathbf{S}_{\hat{\boldsymbol{\Theta}}} = \boldsymbol{E}[(\hat{\boldsymbol{\Theta}}_{ML} - \boldsymbol{\Theta}^*)(\hat{\boldsymbol{\Theta}}_{ML} - \boldsymbol{\Theta}^*)^{\mathrm{T}}] = \mathbf{M}^{-1} \tag{12}$$

where the Fisher information matrix $\mathbf{M}$ is given in terms of the likelihood by

$$\mathbf{M} = \boldsymbol{E}[(\partial \ln L/\partial \boldsymbol{\Theta})^{\mathrm{T}}(\partial \ln L/\partial \boldsymbol{\Theta})]. \tag{13}$$

Since the covariance error matrix for independent Gaussian distributed errors is the same as the asymptotic covariance matrix of any distribution (Goodwin and Payne 1977) it is usual to assume that the errors are Gaussian. Finally, if the model is LP, the parameters are deterministic, and if the errors are additive and independent Gaussian, $\hat{\boldsymbol{\Theta}}_{ML}$ is unbiased and efficient and identical to $\hat{\boldsymbol{\Theta}}_{WLS}$ (see the next section).

If we have little knowledge of the prior distribution of $\boldsymbol{\Theta}$, then its distribution, $f(\boldsymbol{\Theta})$ is very broad with a large variance. In this case the maximum of the *a posterior* probability distribution of $\boldsymbol{\Theta}$, which is the product of the likelihood and $f(\boldsymbol{\Theta})$ will be very close to the maximum of the likelihood function and $\hat{\boldsymbol{\Theta}}_{MAP} \approx \hat{\boldsymbol{\Theta}}_{ML}$.

2.3. Least squares

If the errors are distributed normally with a known variance of $\mathbf{S}_{\mathbf{e}}$, the maximum likelihood method reduces to finding the parameters which minimize

$$(\boldsymbol{z} - F)^{\mathrm{T}}\mathbf{S}_{\mathbf{e}}^{-1}(\boldsymbol{z} - F). \tag{14}$$

† One of the most attractive features of the maximum likelihood method is that if an efficient estimator exists it can always be found by this method.

If the errors have zero mean, these estimates, $\hat{\boldsymbol{\Theta}}_{WLS}$, are unbiased and if the parameters and the data are uncorrelated, the covariance is given by equation (8).

Finally, if the covariance of the errors is diagonal and constant, i.e. $\mathbf{S}_{\mathbf{e}} = \sigma^2\boldsymbol{I}$ (such errors being referred to as *homoskedastic errors*), the estimator $\boldsymbol{\Theta}_{LS}$, called the least squares estimator, is unbiased and the covariance is again given by equation (8). (The corresponding variances for deterministic but unknown parameters using $\hat{\boldsymbol{\Theta}}_{WLS}$ and $\hat{\boldsymbol{\Theta}}_{LS}$ are found by setting $\mathbf{S}_{\boldsymbol{\Theta}}$ to infinity in equation (8).)

If the model is LP, $\hat{\boldsymbol{\Theta}}_{WLS}$ is a minimum variance unbiased estimator, i.e. efficient, and is the best estimator possible. The theory for $\hat{\boldsymbol{\Theta}}_{WLS}$ and $\hat{\boldsymbol{\Theta}}_{LS}$ can be developed without any reference to the statistical properties of the error. In this case, $\hat{\boldsymbol{\Theta}}_{WLS}$ requires only a specification of the weights and these are usually chosen to be the reciprocals of the precision of the readings. When the model is LP and nothing is specified about $f(\boldsymbol{e})$ other than its covariance, $\hat{\boldsymbol{\Theta}}_{WLS}$ is usually termed the Markov least squares estimator.

2.4. Estimation—summary

A preponderance of reported studies use $\hat{\boldsymbol{\Theta}}_{LS}$ or $\hat{\boldsymbol{\Theta}}_{WLS}$, primarily because if the errors are additive, Gaussian, and uncorrelated with the parameters, $\hat{\boldsymbol{\Theta}}_{ML} = \hat{\boldsymbol{\Theta}}_{LS}$ and if $\hat{\boldsymbol{\Theta}}$ is Gaussian, $\hat{\boldsymbol{\Theta}}_{MAP} = \hat{\boldsymbol{\Theta}}_{WLS}$. If the parameter is random, then the correct approach is to use the maximum likelihood approach with $\mathbf{S}_{\boldsymbol{\Theta}}$ being one of the sought after parameters. That is, the model response F must contain $\mathbf{S}_{\boldsymbol{\Theta}}$ explicitly and this may be very difficult to do, either analytically or numerically. Thus it is most common to assume that the parameters are deterministic but unknown, that is, $\mathbf{S}_{\boldsymbol{\Theta}}$ is set to infinity in (8) i.e. no prior information about Θ is available.

Although the maximum likelihood and least squares methods are conceptually simple and their mathematics straightforward, finding the minimum point for nonlinear problems, and most thermal problems are highly nonlinear, can be very difficult and may require regularization† since there tend to be numerous local minima. Solving is often more of an art than a science, especially for biased estimators (Eliason 1993), or if the parameters are constrained (e.g. emissivity must be between zero and one) or when nuisance parameters are present (Nagelkerke 1992). Even for linear problems, as the number of parameters to be estimated increases, the global minimum can be hard to find. We have had success using Powell's method. Fox (1971) gives an excellent summary of the different optimizing methods and some very practical hints about their use. In general, the best approach is a quasi-Newton method, DFP or BFGS (Fox 1971, Press *et al* 1986). Heinkenschloss *et al* (1991) have used grid refinement to stabilize the search for $\hat{\boldsymbol{\Theta}}_{LS}$ but Tai and Neittaanmaki (1991) have demonstrated, when using finite elements, that grid refinement by itself may not suffice and higher order elements may be needed.

† Regularization may be viewed as a form of Bayesian estimation since it is effectively a specification of the prior.

3. Optimal experiment design

It is obvious that the design of the experiment should be strongly influenced by any prior knowledge of $\boldsymbol{\Theta}$ and that the Bayesian approach should be used. But as pointed out previously this method is very difficult to use and optimal designs are generally based upon the maximum likelihood approach assuming that the parameters are deterministic.

If the bias of the estimator is defined by $\boldsymbol{Bi} = \boldsymbol{E}[\hat{\boldsymbol{\Theta}}] - \boldsymbol{\Theta}^*$, the covariance matrix of the error of the estimate is

$$\boldsymbol{E}[(\hat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}^*)(\hat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}^*)^{\mathrm{T}}] = \boldsymbol{Bi}\boldsymbol{Bi}^{\mathrm{T}} + \mathbf{S}_{\hat{\Theta}} \tag{15}$$

and is a combination of the covariance of the estimator and the bias. (Note that this bias is in the estimator and not in the data). Unbiased estimators are clearly preferred, but the bias depends upon the statistics used and it is not always possible to define unbiased statistics. Some investigators have downplayed the importance of the bias, particularly for nonlinear problems, and suggested that an experiment which minimizes the variance is sufficient (Shenton and Bowman 1977). The requirement that the estimator be unbiased can lead to increased errors in the estimated parameters even if $\mathbf{S}_{\hat{\Theta}}$ is a minimum. Norton (1986) shows that a biased estimator based upon ridge regression has a lower parameter error than $\hat{\boldsymbol{\Theta}}_{WLS}$, but in this case the bias is a complex function of $\boldsymbol{\Theta}$ itself which is difficult to determine. If the model is LP, both $\hat{\boldsymbol{\Theta}}_{MC}$ and $\hat{\boldsymbol{\Theta}}_{ML}$ are unbiased. (Although linearizing makes the analysis simpler, it does mean that the solution for $\hat{\boldsymbol{\Theta}}$ is an iterative process involving multiple local extrema.)

The Cramer–Rao theorem establishes a lower bound on the variance of an unbiased estimator $\hat{\boldsymbol{\Theta}}$ of†

$$\boldsymbol{E}[(\hat{\boldsymbol{\Theta}}_{ML} - \boldsymbol{\Theta}^*)(\hat{\boldsymbol{\Theta}}_{ML} - \boldsymbol{\Theta}^*)^{\mathrm{T}}] \geq (\boldsymbol{I} - \partial \boldsymbol{Bi}/\partial\Theta) \times \mathbf{M}^{-1}(\boldsymbol{I} - \partial \boldsymbol{Bi}/\partial\Theta)^{\mathrm{T}}. \tag{16}$$

If $f(\boldsymbol{\Theta}|\boldsymbol{z})$ is Gaussian, the equality holds (Fisher 1922). The Cramer–Rao estimate of the minimum variance is not the only one, but it is convenient in the sense that it can be easily derived from $f(\boldsymbol{z}|\boldsymbol{\Theta})$ and holds for finite sample size. In many cases, the minimum variance is substantially larger than this lower bound. The estimation of the variance of the estimated parameters for small sample sizes is discussed by Shenton and Bowman (1977).

Because the Fisher information approach depends upon conditions which may not be met, e.g. unbiased estimators or large number of samples, LP models, independent identically distributed additive errors, other approaches have been recommended (sensitivity by Knudsen (1994), direct methods by Sinha and Kuszta (1983)). However, the use of $\mathbf{M}$ is widespread, is mathematically convenient and has proven to be an effective approach. Thus even if the estimator is biased and not efficient, we define the optimal experiment as one whose *protocol* minimizes the variance of $\hat{\boldsymbol{\Theta}}$ by maximizing $\mathbf{M}$ through choosing appropriate values of the parameters $\boldsymbol{P}$ in the domain $\boldsymbol{D}$ of all possible values taking special note of any constraints (e.g. conductivity and emissivity must be positive).

† If the parameter is random, then in equation (13) $L = f(\boldsymbol{\Theta}, \boldsymbol{z})$, if it is deterministic but unknown, $L = f(\boldsymbol{z}|\boldsymbol{\Theta})$.

Table 1. Common measures of optimality.

Name	k	$\mathbf{H}$	Formula
D	0	$\boldsymbol{I}$	$(\det(\mathbf{M}))^{1/m}$
A	-1	$\boldsymbol{I}$	$((1/m)\mathrm{trace}\,\mathbf{M}^{-1})^{-1}$
C	-1	$H_{ii} = 1/\theta_i$	$((1/m)\mathrm{trace}\,\mathbf{M}^{-1})^{-1}$
E	∞	$\boldsymbol{I}$	minimum eigenvalue of $\mathbf{M}$
T			trace $\mathbf{M}$
Turing			$1/m\sqrt{\mathrm{trace}\ \mathbf{M}\ \mathrm{trace}\ \mathbf{M}^{-1}}$

If the errors are assumed to be additive and normally distributed with variance $\mathbf{S}$, and if the model is LP and the parameters are deterministic, $\mathbf{M}$ can be expressed by summing over all K data points (Goodwin and Payne 1977)

$$(\mathbf{M})_{lm} = \sum_{k=1}^{K} \left(\frac{\partial F_k}{\partial \Theta_m}\right)^{\mathrm{T}} \mathbf{S}_k^{-1} \left(\frac{\partial F_k}{\partial \Theta_l}\right) + \frac{1}{2}\,\mathrm{tr}\left[\mathbf{S}_k^{-1}\frac{\partial \mathbf{S}_k}{\partial \Theta_l}\mathbf{S}_k^{-1}\frac{\partial \mathbf{S}_k}{\partial \Theta_m}\right] \qquad l, m = 1, \ldots, p. \tag{17}$$

3.1. Optimal criteria

Since $\mathbf{M}$ is a matrix, the optimal experiment design is determined by requiring that some measure $\boldsymbol{\Omega}$ (usually a scalar) of it be a maximum, i.e.

$$\max_{\boldsymbol{P}\in D}\{\boldsymbol{\Omega}(\mathbf{M}(\boldsymbol{P}))\} \Rightarrow \boldsymbol{P}^* \tag{18}$$

where the location of the temperature sensors, sampling times, boundary conditions, etc are defined in the form of a vector $\boldsymbol{P} = \{x_i, y_i, t_j, \ldots\ \boldsymbol{P} \in \boldsymbol{D}\}$.

Whatever the measure used, and there are quite a few depending upon the experiment and the subjectivity of the experimenter, it must satisfy certain conditions, for example we cannot obtain more information by interpolating from two sub-optimal experiments (Pukelsheim 1993). The different measures most commonly used for the optimization of the experimental conditions are of the form (Walter and Pronzato 1990, Pazman 1986)

$$\begin{aligned} &\text{if } \det(\mathbf{M}) \neq 0 \qquad \boldsymbol{\Omega} = [m^{-1}\mathrm{trace}(\mathbf{H}\mathbf{M}^{-1}\mathbf{H}^{\mathrm{T}})^k]^{1/k} \\ &\text{if } \det(\mathbf{M}) = 0 \qquad \boldsymbol{\Omega} = \infty \end{aligned} \tag{19}$$

where $\mathbf{H}$ is a non-singular $m \times m$ matrix and where $k \geq 0$. Table 1 lists several measures and their common names. The most common optimality criterion is D-optimality and its appeal is that it corresponds to minimizing the volume of the ellipsoid which represents the maximum confidence region for the maximum likelihood estimate of the unknown parameters when $\mathbf{S}(\boldsymbol{e})$ is unknown. If one parameter has a very large variance compared to the others, the confidence ellipsoid will be skinny and long and minimizing its volume may be misleading. In this case, E-optimality, which maximizes the minimum diameter of the ellipsoid, or the Turing optimality which tries to make the ellipsoid a sphere, are preferable. Both D- and E-optimalities are difficult to compute and C-optimality† which minimizes the sum of the variances (sometimes

† C-optimality is equivalent to A-optimality if the parameters are non-dimensionalized

referred to as the generalized variance) is often used because of its mathematical simplicity. G-optimality, which seeks to maximize the minimum information over the entire domain $\boldsymbol{D}$, is equivalent to D-optimality if $\mathbf{S}_e$ is constant over the readings, i.e. white noise. T-optimality, which produces $\hat{\boldsymbol{\Theta}}_{ML}$ when $\mathbf{S}(\boldsymbol{e})$ is known, is a very weak and unsatisfactory optimality (Pukelsheim 1993).

When only one parameter is sought, $\mathbf{M}$ is a scalar, and all of these criteria are equivalent. When more than one parameter is sought, the different criteria will differ in numerical value. Regardless of which optimality criterion is used, the minimum value of $\boldsymbol{\Omega}$ can be found in two ways. First, by enumerating the values of $\boldsymbol{\Omega}$ at all possible parameters and visually searching for the minimum, and second, by using a nonlinear minimizing program. We have used both methods, employing NPSOL (Gill 1986) as the minimizing program. Although the problem of locating the minimum of $\boldsymbol{\Omega}$ appears to be rather straightforward, we found the same numerical difficulties discussed above in section 2.4.

It is important to note that the use of $\mathbf{M}$ requires some knowledge about the noise of the readings, but requires no knowledge about the measured data. It must be emphasized that the elements of the information matrix $\mathbf{M}$ depend on the *a priori* estimates of the unknown parameters $\boldsymbol{\Theta}$ because of the strongly nonlinear dependence of the temperature on the unknown parameters and this is typical of measurement designs for the solution of inverse problem in thermal–structural problems. Accordingly, it is only meaningful to speak of locally optimal designs, which are formulated with the use of *a priori* information about the unknown parameters.

3.2. Prior knowledge

If the parameter is random (e.g. the conductivity of a heterogeneous material) and some information is available about its distribution, the Bayesian cost or MAP estimators are appropriate. However, in view of the mathematical difficulties in evaluating $\hat{\boldsymbol{\Theta}}_{MC}$ and $\hat{\boldsymbol{\Theta}}_{MAP}$, determining the optimal protocol is almost impossible. Walter and Pronzato (1987) have studied incorporating prior knowledge by maximizing the expected values of the D-optimality measures of $\mathbf{M}$ or minimizing the expected values of $\mathbf{M}^{-1}$ where the expectation is evaluated over all θ. These two criteria are not equivalent when $\mathbf{M}$ is a function of θ and they found that the corresponding protocols were significantly different.

3.3. Extended Fisher information matrix

When there are uncertainties in some of the parameters $\boldsymbol{b}$, for example in the surface heat transfer coefficients, Fadale *et al* (1995) have shown that an appropriate extension of $\mathbf{M}$ is

$$(\mathbf{M})_{lm} = \sum_{k=1}^{K} \left[\left\{ \frac{\partial F_k}{\partial \Theta_m} \right\}^{\mathrm{T}} \boldsymbol{\Sigma}_k^{-1} \left\{ \frac{\partial F_k}{\partial \Theta_l} \right\} + \frac{1}{2} \operatorname{tr} \left[\boldsymbol{\Sigma}_k^{-1} \frac{\partial \boldsymbol{\Sigma}_k}{\partial \Theta_l} \boldsymbol{\Sigma}_k^{-1} \frac{\partial \boldsymbol{\Sigma}_k}{\partial \Theta_m} \right] \right] \qquad l, m = 1, \ldots, p \tag{20}$$

where the extended covariance matrix $\boldsymbol{\Sigma}_k$ is defined as

$$\boldsymbol{\Sigma}_k = \mathbf{S}_k + \left(\frac{\partial F}{\partial \boldsymbol{b}} \right) \mathbf{G} \left(\frac{\partial F}{\partial \boldsymbol{b}} \right)^{\mathrm{T}} \tag{21}$$

and $\mathbf{G}$ is the covariance matrix of the uncertain parameters†. The details of the calculation of $\boldsymbol{\Sigma}$ are given in Fadale *et al* (1995).

If there are no uncertainties in the *known* parameters $\boldsymbol{b}$, then $\mathbf{G}$ is identically zero, $\boldsymbol{\Sigma}_k \equiv \mathbf{S}_k$ and the likelihood reduces to the usual form, equation (17), which is dependent only upon the noise. In many of the cases we have studied, $\mathbf{M}$ is only weakly affected by the trace term. In this situation, a comparison of equations (17) and (20) suggests that $\boldsymbol{\Sigma}_k$ can be considered as the equivalent noise of the experiment. Even if the signal noise is independent of time, the equivalent noise is a strong function of time through the term $\partial F/\partial \boldsymbol{b}$.

4. Examples

In the following examples, the information is computed by using equation (20) applied at specific locations, i.e. for only one or two temperature sensors, ignoring the trace term, and evaluating the terms in the summation at equally spaced increments of time. For only one sensor, the variance $\mathbf{S}$ is a scalar and equal to the variance of the measured temperature, $\sigma^2(T)$. For multiple sensors, we assume that the errors of the two sensors are uncorrelated, i.e. $\mathbf{S} = \sigma^2(T)\boldsymbol{I}$. In the case where we examine the effect of uncertainty in the heat transfer coefficient, cases IV, VI, and VII, the extended covariance matrix $\mathbf{G}$, equation (21), is also a scalar and equal to $\sigma^2(h)$. In all cases, the derivatives at each sensor, $\partial T/\partial\theta$ and $\partial T/\partial \boldsymbol{b}$ are evaluated either analytically or by finite differencing the temperatures computed by a finite element program (Haftka 1981, Emery and Fadale 1998b).

If the bias is constant, according to the Cramer–Rao theorem, equation (16), using an appropriately non-dimensionalization, $\mathbf{M}$ is a lower limit on the uncertainty of the estimated parameter

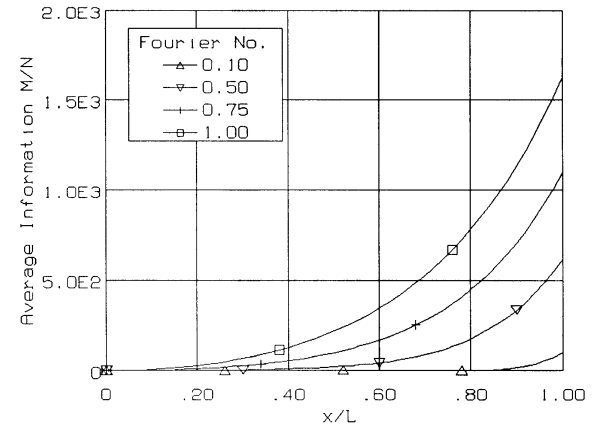
$$\frac{\sigma^2(\theta)}{\theta^2} \geq \mathbf{M}^{-1}. \tag{22}$$

Since $\mathbf{M}$ increases with the number of readings, it is always possible to reduce the variance to any level by taking enough readings. For this reason, the appropriate measure of the effectiveness of an experimental protocol is best measured by the average information per reading, $\mathbf{M}/N$, not by $\mathbf{M}$.

4.1. 1D heat flow

Let us study the problem of estimating the thermal conductivity of a homogeneous material by a series of experiments involving one-dimensional heat flow through a slab of thickness L. The initial temperature is T_0 and

† $\mathbf{G}$ will not be diagonal if $\boldsymbol{b}$ are correlated, for instance if $\boldsymbol{b}$ represent several surface heat transfer coefficients which are dependent upon a common fluid velocity.



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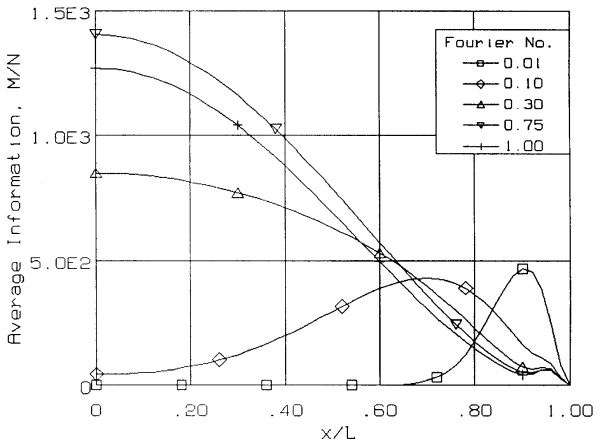
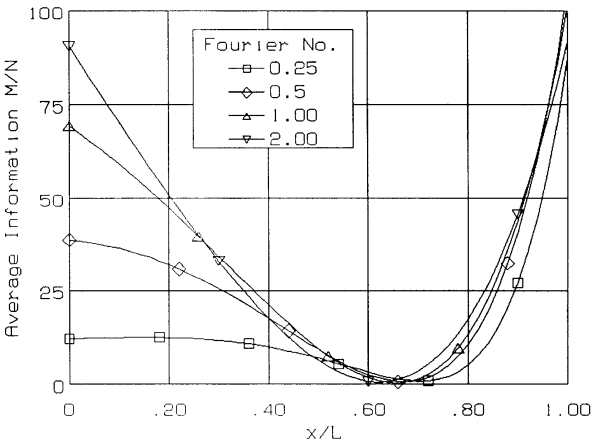


(*b*)

Figure 1. (*a*) Average information for case I (applied heat flux) when sensing temperature. (*b*) Average information for case I (applied heat flux) when sensing heat flux.



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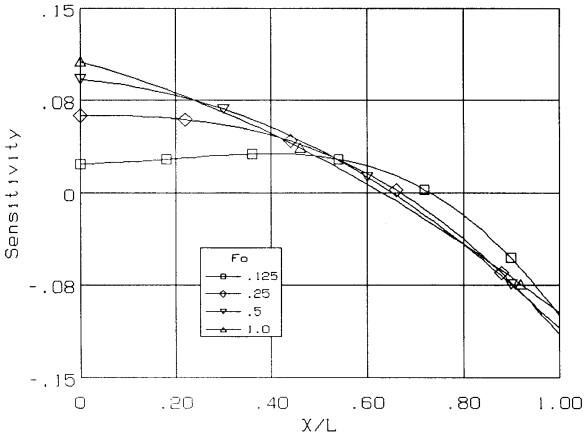


(*b*)

Figure 2. (*a*) Average information for case II (convective boundaries). (*b*) Sensitivity of temperature $(\partial T/\partial k)$ for case II.

the density and specific heat capacity are 100 kg m^{-3} and 10 000 kJ $kg^{-1}\,°C^{-1}$. The nominal thermal conductivity is 10 W $m^{-1}\,°C^{-1}$. Temperatures and heat fluxes will be measured at equal time intervals over the duration of the experiment. The measurements will be have a noise, $\sigma(T)/T_{maximum}$ and $\sigma(q_x)/Q$ of 1%.

4.1.1. Case I: applied heat flux. Let the temperature at $x = 0$ be fixed at the value T_0 and let a constant heat flux Q be applied at $x = L$ such that the steady state temperature at $x = L$ is $T_0 + 100\,°C$. Figure 1(*a*) shows the average information per reading for temperatures measured at different values of x and for different experimental durations (time is expressed in terms of the Fourier number, $Fo = kt/\rho cL^2$; a value of 10.0 is essentially steady state). The information at $x = 0$ is always zero because the temperature is fixed and is thus independent of k. As expected, the greatest information is obtained from temperatures measured at the heated surface and this information continually rises with time until it reaches a maximum at steady state of 6400. The values shown at $Fo = 1.0$ are substantially less than this steady state value because the information conveyed by the earlier samples is so much less.

Figure 1(*b*) shows the information from measuring the heat flux. Here the point of maximum information follows the thermal pulse as it moves from the heated surface towards the cooled surface. When $Fo > 0.75$ the heat flux at $x = 0$ has increased to the point that measurements made there convey the greatest information. At steady state, $q_x = Q$, a constant, and the information about the conductivity is zero. This effect of reduced information as the steady state is approached is illustrated by the curve for $Fo = 1.0$ for which the values of $\mathbf{M}/N$ are less than for $Fo = 0.75$. This behaviour in which the information is maximum at an intermediate time is common in thermal problems. Figure 1(*b*) clearly indicates that there is an optimal sensor location, e.g. the values of x for which $\mathbf{M}$ is a maximum, and that this optimal point varies with the duration of the experiment.

4.1.2. Case II: convective heating at $x = L$. If instead of applying a constant heat flux at $x = L$, the surface is subjected to convective heating with a fluid

Table 2. Average information **M** when determining k based upon sensors located at the optimal positions. Noise = 1%, no uncertainty in known parameters.

Fo	Boundary conditions				
$x = 0$	$T = T_0$	$T = T_0$	$T_\infty = T_0 + 100\,^\circ$C $Bi = 0.8$	$T_\infty = T_0$ $Bi = 0.2$	$T_\infty = T_0$
$x = L$	$q_x = Q$	$T = T_L$	$T_\infty = T_0 + 100\,^\circ$C $Bi = 0.8$	$T_\infty = T_0 + 100\,^\circ$C $Bi = 0.8$	$T_\infty = T_0 + 100\,^\circ$C $Bi = 0.8$
0.01	11	17	9	9	99
0.05	52	18	31	32	32
0.10	103	17	46	52	52
0.50	617	17	37	100	149
0.75	1099	17	40	87	211
1.00	1613	17	38	90	267
∞	6400	0	0	91	610

temperature $T_\infty = T_0 + 100\,^\circ$C, the temperature and heat flux distributions are very similar to those of case I and the information history is qualitatively similar. However the magnitude of the information is different as indicated in the last column of table 2.

Table 2 also shows the information available for several different boundary conditions. In general, we have found that applied flux boundary conditions provide the most information. In many thermal experiments, the steady state temperature may not be as strong a function of the parameter sought as some intermediate temperature. If the boundary conditions are symmetric, column 4 of table 2, then the steady temperature is completely independent of k, and the most information is gained at an intermediate time, see column 5. The results shown in column 6 indicate that: (a) the early time information is greatest ($Fo = 0.0$) and reduces thereafter as the temperature field penetrates into the slab and the surface temperature becomes relatively constant with respect to time; (b) at later times the optimal sensor location moves away from the convective boundary and it is possible to find a location of high information, $Fo \geq 0.5$.

4.1.3. Case III: convective heating at $x = 0$ and L. Since it is experimentally difficult to maintain a surface at a fixed temperature, let us consider the case where the surface at $x = 0$ is exposed to a fluid of temperature T_0 with the same heat transfer coefficient as at $x = L$. Figure 2(a) shows the information history and it is very different qualitatively and quantitatively from cases I and II. At early times, the information history near $x = L$ is essentially the same as in case I. However, the information provided by measuring the temperature near $x/L = 0.7$ is near zero at all times. Meanwhile the temperature rise at $x = 0$, which begins about $Fo = 0.1$, becomes informative for $Fo > 0.25$ and at steady state provides nearly as much information as the temperature measured at $x = L$. The information at $x = L$ shows a slight peak in time at about $Fo = 1.0$ and a small reduction thereafter.

The dearth of information near $x/L = 0.7$ is because, for the specific boundary conditions and conductivity, the temperature there is quite insensitive to the conductivity, i.e. the sensitivity $\partial T/\partial k \approx 0$ and from equation (17)

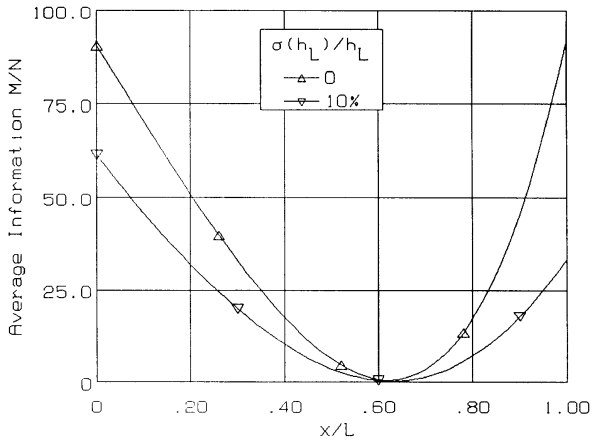


Figure 3. The effect of uncertainty in the convective heat transfer coefficient.

M is proportional to the sensitivity squared. Figure 2(b) shows how the sensitivity remains small in this region over the entire experiment. This lack of sensitivity is equivalent to the loss of identifiability mentioned in the introduction. Although we observed this feature through numerical experimentation, Musylev (1980) and Kurzhanski and Khapalov (1991) have investigated this question of observability and sensitivity in a more general way and developed mathematical conditions under which sensors will give negligible information in conduction problems. In the steady state, if the convection coefficients are equal at both surfaces, the temperature at the centre of the plate is independent of the conductivity, while that at the surfaces is strongly conductivity dependent. The result is the near quadratic profile shown in figure 2(a).

4.1.4. Case IV: convective heating with uncertainty in the convection coefficients. If there is uncertainty in the surface heat transfer coefficient at $x = L$, then it is intuitive that the information provided by the experiment will be degraded. The available information can be found by applying (20) with the uncertain parameter b being h_L. Figure 3 compares the information with 10% uncertainty

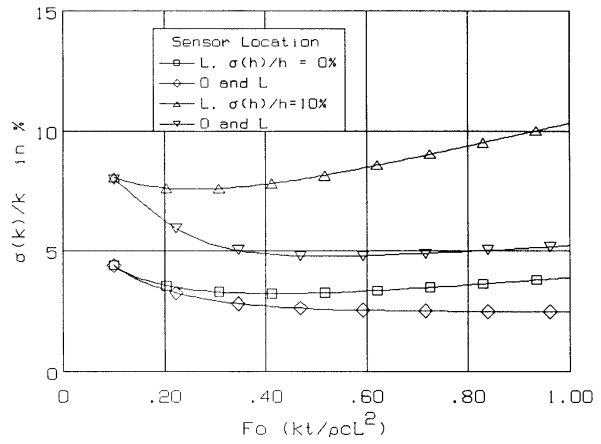


Figure 4. The effect of multiple sensors and uncertainty in convection on $\sigma(k)/k$ as a function of the duration of the experiment.

in h_L to that of zero uncertainty and the information is reduced at all values of x. However, the effect is greatest at $x = L$, but less at $x = 0$ where the temperature is more sensitive to the boundary condition at $x = 0$ than to that at $x = L$. More importantly, the optimal sensor location has moved from $x = L$ to $x = 0$, and this is true for durations of the experiment exceeding $Fo = 0.25$.

4.1.5. Case V: insulated surface and multiple sensors. Finally, we examine the case where the surface at $x = 0$ is insulated and convection occurs at $x = L$. In the steady state the temperature will be equal to T_∞ everywhere, independent of k, so that the information provided by this experiment will be zero at long times. However, the steady state is achieved very slowly compared to the case where there is convection at $x = 0$, and up to $Fo = 2$, there is ample dependence of temperature upon k to acquire some useful information. While the information at $x = L$ is about one quarter of that for the case where there is convection at $x = 0$, the information obtained by measuring the temperature at $x = 0$ is about the same. Figure 4 shows the time variation in the minimum standard deviation of the estimated conductivity as a function of the experiment duration, assuming that only a total of ten measurements are made.

We see that there is a steady erosion of accuracy if only data from $x = L$ is used. If two sensors are used, then the additional information which comes from the sensor at $x = 0$ at later times results in an almost constant accuracy of estimation of about 2%. If there is a 10% uncertainty in the convective coefficient at $x = L$, the second sensor becomes critically important since it is far enough from the affected boundary to be relatively unaffected by uncertainty in h_L. Here, relying only on the sensor at L will result in a very inaccurate experiment, with estimated errors of 10% for the longest experiment. But by using two sensors, the accuracy remains nearly constant at 5% and is not significantly worse than the case of zero uncertainty in h_L.

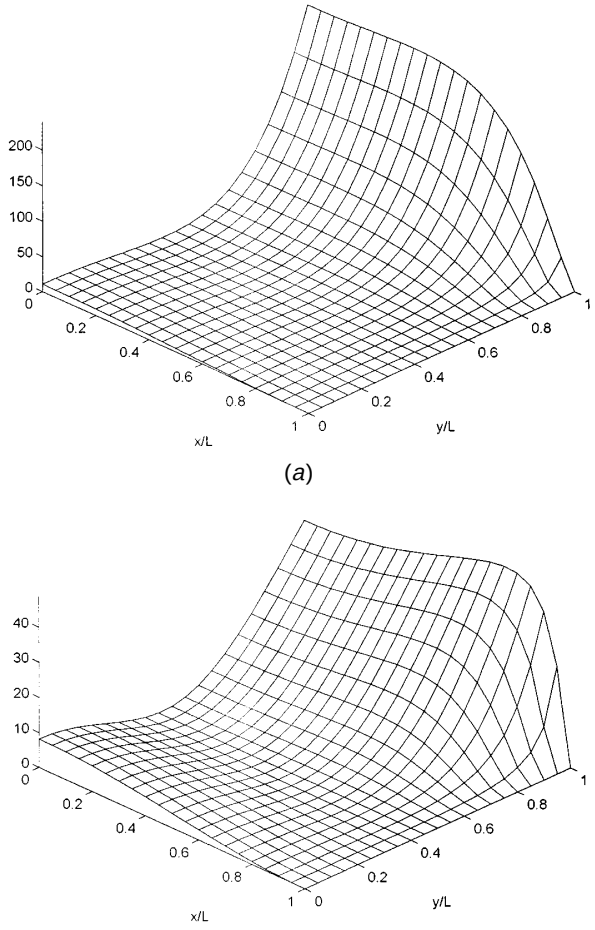
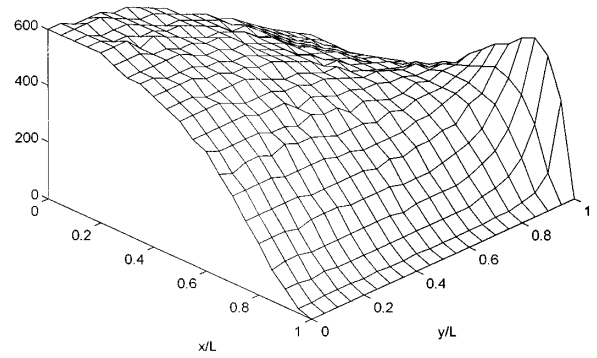


Figure 5. (*a*) Information profile for 2D problem at *Fo* = 0.50. (*b*) The effect of uncertainty in convection for the 2-D problem at *Fo* = 50.

4.2. 2D heat flow

4.2.1. Case VI: two dimensional conduction. Consider the two-dimensional analogue to Case II. A region, $L \times L$, is initially at T_0 with insulated edges at $x = y = 0$, a fixed temperature of T_0 at $x = L$ and convection at $y = L$ to a fluid with a convective coefficient h_L and a fluid temperature of $T_\infty = T_0 + 100\,^\circ$C. Figure 5(*a*) shows the information at steady state as a function of temperature location. There is little information available near $x = L$ because of the fixed temperature. Likewise, the small temperatures near the lower corner, $x = y = 0$, convey little information. The optimal location for a sensor is at $x = 0$, $y = L$, where the heat flux is relatively unaffected by the fixed temperature boundary. Here the quantity of information is equal to that of Case II at steady state, table 2. Figure 5(*b*) illustrates the effect of a 10% uncertainty in the heat transfer coefficient. There has been a significant loss of information and now the optimal sensor location is no longer clearly defined.

It should be noted that while the steady state information map is the same whether $T_\infty = 100$ and $T_0 = 0$



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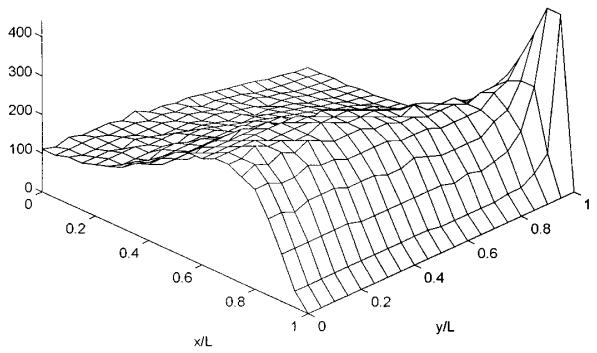

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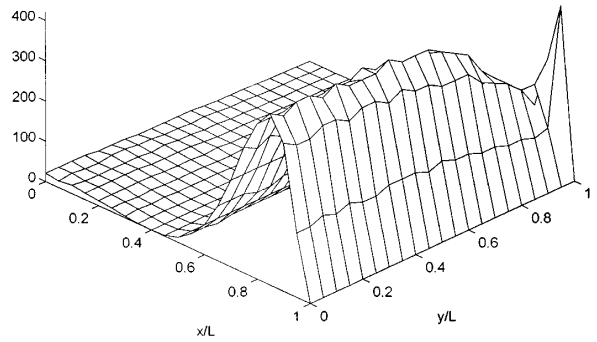
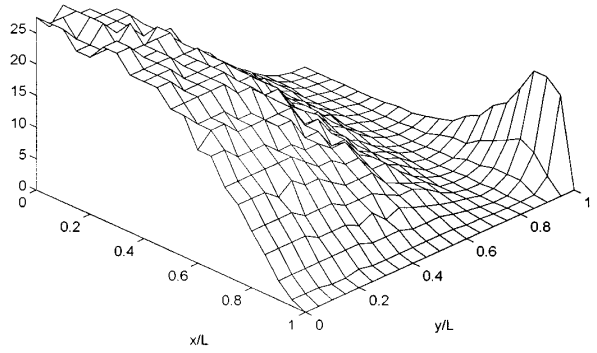


(*c*)

Figure 6. (*a*) Information profile for 2-D problem with surface convection when estimating k for $2h_S L/h_L t = 2.5$. (*b*) Information profile for 2-D problem with surface convection when estimating k for $2h_S L/h_L t = 5.0$. (*c*) Information profile for 2-D problem with surface convection when estimating k for $2h_S L/h_L t = 10.0$.



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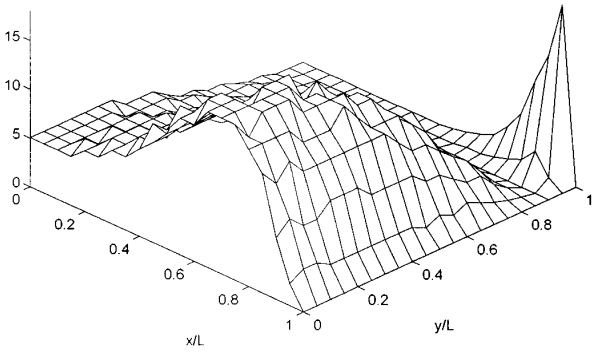

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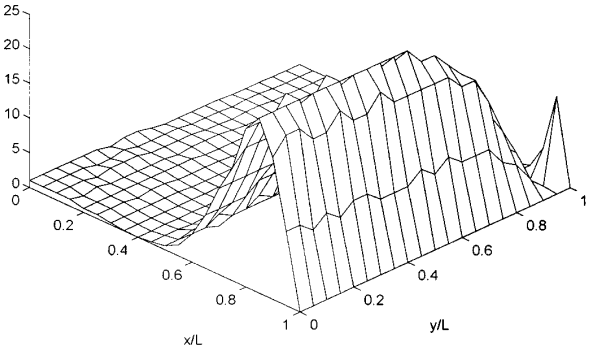

(*c*)

Figure 7. (*a*) Information profile for 2-D problem with surface convection when estimating h_S for $2h_S L/h_L w = 2.5$. (*b*) Information profile for 2-D problem with surface convection when estimating h_S for $2h_S L/h_L w = 5.0$. (*c*) Information profile for 2-D problem with surface convection when estimating h_S for $2h_S L/h_L w = 10.0$.

or $T_\infty = 0$ and $T_0 = 100$, the transient behaviour is very different. If the heating comes from T_0 then the optimal sensor location moves along $y = 0$ from $x = L$ to $x = 0$ and then upward along $y = 0$ to the corner $x = 0$, $y = L$. If the heating is applied at the convective boundary, the optimal sensor location is at $x = 0$, $y = L$ for all times.

4.2.2. Case VII: surface convection. Let us extend Case VI by assuming that the region $L \times L$ represents a plate of thickness w with convection from both the upper and lower surfaces with a convective coefficient of h_S and an ambient temperature equal to that associated with the edge $y = L$. Now the temperature field is a function of both the edge Biot number, $h_L L/k$ and the ratio of the surface conductance and the edge conductance, $h_S 2L^2/h_L Lw = 2h_S L/h_L w$. When the plate is thick, the surface heat loss has little effect on the temperature profile and the information map is qualitatively similar to figure 5(*a*), but with a peak value of approximately 600. As the thickness is reduced, the surface heat transfer begins to dominate. Figure 6 shows the information map for values of $2h_S L/h_L w$ of 2.5, 5, and 10. The optimal sensor location, at steady state, is seen to be a strong function of plate thickness, but sensors placed along the edge $y = L$ would yield reasonable estimates of the thermal conductivity.

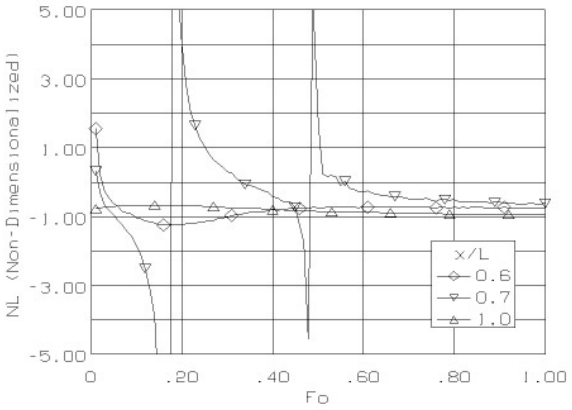

Figure 8. Nonlinearity with respect to k for Case III.

If one wished to estimate the value of h_S, the situation is very different, figure 7. Here the information content is very small ≈25 and there is no single best sensor location.

4.3. Linearity

Almost all of the theoretical results for optimal estimation and experimental design are based upon the LP model. While the behaviour of thermal systems with constant properties is linear in applied boundary temperatures and heat fluxes over the duration of the experiment, it is rarely linear in the conductivity or convection coefficients.

Let us express F (appropriately non-dimensionalized) as

$$F(\Theta) = F(\Theta') + \left.\frac{\partial F}{\partial \Theta}\right|_{\Theta'} (\Theta - \Theta') + \frac{1}{2}\left.\frac{\partial^2 F}{\partial \Theta^2}\right|_{\Theta'} (\Theta - \Theta')^2 \ldots \tag{23}$$

and define a non-dimensional nonlinearity (NL) per unit $(\Theta - \Theta')/\Theta'$ as

$$NL = \frac{\theta}{2} \left.\frac{\partial^2 F/\partial \Theta^2}{\partial F/\partial \Theta}\right|_{\Theta'}. \tag{24}$$

Figure 8 shows the time history of NL for three sensor locations for Case III. If we arbitrarily require that the second-order term in (23) be less than 0.1 and that we are capable of locating Θ' within 10% of Θ^*, then $|NL|$ must be less than 1. $\partial^2 T/\partial \Theta^2$ is well behaved at all times and at all sensor locations, so the behaviour of NL is primarily due to that of $\partial T/\partial \Theta$. Sensors which are near $x/L = 0.7$ where $\partial T/\partial k$ is near zero at all times, figure 2(*b*), show substantial amounts of nonlinearity while those away from this region are well behaved and LP in nature. If problem sensor locations and measurements are excluded in our analysis, then from figure 8 we can see that nonlinearity is never a problem. Because **M** is a direct function of $\partial T/\partial \Theta$ the occurrence of strong nonlinearities is coincident with loss of information and also, therefore, of identifiability. Thus if one avoids sensor locations and times which do not contribute to **M**, at least for all of the thermal examples given here, nonlinearity is not a matter of concern.

5. Conclusions

The examples have demonstrated the use of the Fisher information matrix to design experiments which maximize the available information. Although we have described only a very simple application, it is clear that with modern computational tools (e.g. finite elements) the calculation of **M** can be done with relative ease even when there are uncertain parameters. Emery *et al* (1997) and Emery and Fadale (1998a) have applied the extended Fisher matrix to study the effect of imprecision in boundary conditions, sensor location, and sampling times. They have also studied the simultaneous estimation of conductivity and specific heat capacitance. Although Artyukhin (1985) recommended the use of D-optimality, Emery and Fadale (1997) demonstrated that when the sensitivities $\partial T/\partial k$ and $\partial T/\partial c$ behave oppositely with time, E-optimality is preferable.

While we have treated only thermal problems, the method has been used by others in a wide variety of studies. Rafajlowicz (1981) discusses the optimal input signal and sensor location to estimate the eigenvalues of linear parabolic pdes. Gevers and Ljung (1986) review the optimal design when the simulating equations are not exact using transfer functions. Leontaritis and Billings (1987) examined nonlinear systems and point out that an experiment which is optimal for a linear system may lead to substantial errors and loss of identifiability when applied to nonlinear systems. They point out that good experiments require *a priori* knowledge of θ which is rarely available, thus forcing the experimenter to evaluate **M** for a range of θ just as we have done in the examples.

Witkowski and Allen (1993) investigated nonlinear truss sytems and the linearization necessary to estimate the parameters and drew conclusions similar to those we have discussed in the preceeding section. Bayard *et al* (1988) examined a large flexible space structure to identify modal frequencies and damping parameters. Using the D-optimality they showed that the excitation signal could be decoupled from the sensor locations.

Taktak *et al* (1993) studied the effect of sensor location, experiment time, and geometry on the determination of the thermal properties of composites. Vozar and Groboth (1997) used the ideas of optimal experiment design to determine the relative performance of step heating and laser flash methods when estimating the thermal diffusivity of poorly conductive materials. On the opposite tack, Pritchard *et al* (1996) used these ideas to optimize a structure so that it was minimally sensitive to those parameters which the designers were least confident of.

This series of examples clearly differentiates the different experiments on the basis of boundary conditions, measurement times, sensor location, and whether to measure temperature or heat flux and permits the experimenter to choose the best experiment by comparing the information obtained with the cost of the measurements. These conclusions are relatively easy to draw when only one sensor is used. For multiple sensors, it is not so easy. One must evaluate the total information provided by both sensors as they range through all possible locations. In

the 1D experiment this is not too difficult since realistic measurement points are only at $x = 0$ and L. For a 2D experiment, measurements can be made over the entire plate and finding sensor locations which maximize the information is numerically difficult. In the example given here, locating the sensors is easy because of the shape shown on figure 4(a). However, more difficult experiments often show several local maxima for one sensor.

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