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# Uncertainties in parameter estimation: the inverse problem

TUSHAR D. FADALE
Department of Aeronautics and Astronautics, University of Washington, Seattle, WA 98195, U.S.A.

ALEKSEY V. NENAROKOMOV
Department of Space System Engineering, Moscow Aviation Institute, Moscow, Russia

and

ASHLEY F. EMERY†
Department of Mechanical Engineering, University of Washington, Seattle, WA 98195, U.S.A.

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**Abstract**—The procedure of parameter estimation and the parameter estimates are not only affected by the measurement noise, which is present during any experiment, but are also influenced by the known model parameters. The most commonly used functional, which is based on the maximum likelihood principle, only accounts for the experimental noise but not the effect of the uncertainties in the known parameters. A new functional for parameter estimation has been proposed, which will also take into account the uncertainties in the known model parameters. It is shown that, in the presence of uncertainties in the known model parameters, the proposed functional is superior to previous functionals.

## INTRODUCTION

At the current time two topics of emphasis in the study of heat and mass transfer processes are: (1) the development of analytical/computational models based on quite intricate theories; and (2) the improvement of the methodology of experimentation to simulate the natural process. The basic goal of both these topics is to simulate the responses of processes as accurately as possible. The inverse method combines these two approaches: relying on experimental measurements to validate the mathematical model. Using the inverse method, improved estimates of properties or parameters of the mathematical model are possible. The mathematical model of a certain physical process is usually taken to be a set of differential equations with known and unknown coefficients. It can be suggested that the structure of the mathematical model is known, but that the parameters are either not known or are known only approximately. The additional information necessary for the inverse problem is the experimental observation of the state of the model (for example the temperature). The inverse problem can then be considered as a problem of identifying the unknown parameters of the mathematical model by minimizing a specific measure of performance.

One of the first of such methods is the least-squares technique, suggested by Legendre [1], in which the sum of the squares of the differences between the experimental measurements and the calculated responses of the system is minimized. This approach is based on a deterministic view of the system. Additional measures of performance have been based on a stochastic description of the experimental noise. The estimates obtained from this latter approach are referred to as the maximum likelihood estimates. A number of practical applications of parameter estimation, based upon both approaches, have been in the fields of controls and hydrology. A comprehensive review of these techniques is given by Polis [2]. Recent years have seen applications of parameter estimation techniques to heat and mass transfer processes [3–5].

Although all the above-mentioned approaches consider the experimental noise to be stochastic, few of them take into account errors or uncertainties which might exist in the known parameters of the system. This paper presents a generalization of the inverse method which permits the estimation of the parameters when the known parameters are variables and are statistically related. The following sections develop the theory and give several examples of its use. In addition to parameter estimation, considerable emphasis has been given to the design of optimal experiments. A good survey of the techniques is given by Kubrusly and Malebranche [6]. A following paper

†Author to whom correspondence should be addressed.

## NOMENCLATURE

| | |
|---|---|
| **b** | known parameter vector |
| *Cov* [ ] | covariance operator |
| *E*[ ] | expected value operator |
| *f* | probability density function |
| **G** | covariance matrix of known parameters |
| *h* | heat transfer coefficient |
| *J* | proposed likelihood functional |
| *k* | thermal conductivity |
| *K* | number of observation times |
| *L* | likelihood functional |
| *N* | number of sensors |
| N[0, 1] | normally distributed random number with 0 mean and 1 standard deviation |
| *P* | number of parameters |
| **q** | eigenvector |
| **Q** | orthogonal matrix of eigenvectors |
| **S** | covariance matrix of temperature measurement |
| *t* | time |
| $T_\infty$ | ambient temperature |
| **u** | unknown parameter vector |
| *Var* [ ] | variance operator |
| **V** | covariance matrix of temperature |
| *x*, *y* | sensor position |
| **X** | vector of sensor positions |
| **z** | measured temperature vector. |

Greek symbols

| | |
|---|---|
| $\Gamma$ | least square functional |
| $\delta_h$ | percentage variation in *h* |
| $\delta_n$ | percentage variation in measurements |
| $\boldsymbol{\Theta}$ | sensitivity matrix of the state of the system to **b** |
| $\lambda$ | eigenvalue |
| $\boldsymbol{\Lambda}$ | diagonal matrix of eigenvalues |
| $\sigma_h$ | standard deviation of *h* |
| $\sigma_n$ | standard deviation of measurements |
| $\boldsymbol{\Phi}$ | predicted temperature vector |
| $\boldsymbol{\Psi}$ | discrepancy between prediction and measurement vector. |

Subscripts

| | |
|---|---|
| *i*, *j* | sensors |
| *k* | time |
| *l*, *m* | parameters. |

Superscript

| | |
|---|---|
| T | transpose. |

will discuss the issue of optimal experiment design in relation to this new criterion.

## THEORY

Consider a thermal system which can be modelled by a set of differential equations and model parameters. Of all the parameters involved in the model, let there be *P* unknown parameters represented by the vector **u**, while the rest of the parameters (say *Q* parameters) are known *a priori* and are represented by the vector **b**. In order to estimate the parameters, i.e. **u**, experimental observations of the responses of system are obtained at various locations $(x_i, y_i)$ and times $(t_k)$, none of which need be uniformly spaced. Let *N* be the number of sensors used in the experiment and *K* the number of readings in time at these sensor locations. Then the experimental observations can be represented by $\mathbf{z}_k$ where,

$$\mathbf{z}_k^{\mathrm{T}} = [z_i(t_k), i = 1, 2, .., N] \quad k = 1, 2, \ldots, K. \quad (1)$$

In practice, the unknown parameters are estimated by minimizing a criterion expressed in terms of the *residuals*, where the residuals are the differences between the predicted responses of the system and the experimentally observed responses at the sensor locations and the sample times. Broadly speaking, there are two approaches to define this criterion, the least squares approach and the maximum likelihood approach.

In the least squares approach to the inverse problem, the unknown parameters, **u**, are estimated by minimizing the sum of the squares of the residuals, i.e. minimize $\Gamma(\mathbf{u})$ where $\Gamma$ is given as:

$$\Gamma(\mathbf{u}) = \sum_{k=1}^{K} (\boldsymbol{\Phi}_k - \mathbf{z}_k)^{\mathrm{T}} (\boldsymbol{\Phi}_k - \mathbf{z}_k), \quad (2)$$

and $\boldsymbol{\Phi}_k$ is a vector of the predicted responses of the system at all the sensor locations based on the mathematical model. For distributed parameter systems this involves the solution of the field equations:

$$\boldsymbol{\Phi}_k^{\mathrm{T}} = [\phi(x_i, y_i, t_k), \quad i = 1, 2, .., N] \quad k = 1, 2, \ldots, K. \quad (3)$$

where $x_i$, $y_i$ is the location of the *i*th sensor and $t_k$ is the *k*th sample time.

In the maximum likelihood approach, the problem is considered from a probabilistic point of view. The experimental measurements of the responses of the system are considered to be random in nature and the measurement errors are assumed to be spatially and temporally independent of each other and to be normally distributed with a zero mean and a variance of $\sigma_n^2$. This randomness exists only in the measured responses **z** (because of the experimental noise) and not in the predicted responses, $\boldsymbol{\Phi}$, because the mathematical model of the system was taken as deterministic. The best estimates of the unknown parameters are those which maximize the likelihood of

occurrence of the measurements relative to the predictions. In other words, the best estimate is that which maximizes the probability density function of the measurements $f(\mathbf{z}|\mathbf{u})$. This estimate of $\mathbf{u}$ makes the measurement *most likely* and therefore the probability density function $f(\mathbf{z}|\mathbf{u})$ is called the likelihood function, given by:

$$f(\mathbf{z}|\mathbf{u}) = \left[(2\pi)^{NK}\prod_{k=1}^{K} Det\,(\mathbf{S}_k)\right]^{-1/2} \times \exp\left\{\sum_{k=1}^{K} -\tfrac{1}{2}[\mathbf{\Phi}_k(\mathbf{u})-\mathbf{z}_k]^{\mathrm{T}}\mathbf{S}_k^{-1}[\mathbf{\Phi}_k(\mathbf{u})-\mathbf{z}_k]\right\}, \quad (4)$$

where $\mathbf{S}_k$ is the covariance matrix of the measurements at time $t_k$ and is defined as:

$$\mathbf{S}_k = E[\delta\mathbf{z}_k\,\delta\mathbf{z}_k^{\mathrm{T}}] \quad \delta\mathbf{z}_k = \mathbf{z}_k - E[\mathbf{z}_k]. \quad (5)$$

Because of the exponential character of the density function it is convenient to deal with the logarithm of the likelihood function. The criterion for the estimation of the unknown parameters $\mathbf{u}$ is therefore defined by the likelihood functional $L^*$:

$$L^* = -2\ln f(\mathbf{z}|\mathbf{u}) = NK\ln(2\pi) + \sum_{k=1}^{K}\ln\,[Det\,(\mathbf{S}_k)] + \sum_{k=1}^{K}[\mathbf{\Phi}_k(\mathbf{u})-\mathbf{z}]^{\mathrm{T}}\mathbf{S}_k^{-1}[\mathbf{\Phi}_k(\mathbf{u})-\mathbf{z}_k], \quad (6)$$

where the best estimates of $\mathbf{u}$ will minimize the likelihood functional, $L^*$. Assuming that the experimental noise is independent of the unknown parameters, the first two terms are constants and the minimization of $L^*$ is equivalent to the minimization of $L$:

$$L = \sum_{k=1}^{K}[\mathbf{\Phi}_k(\mathbf{u})-\mathbf{z}_k]^{\mathrm{T}}\mathbf{S}_k^{-1}[\mathbf{\Phi}_k(\mathbf{u})-\mathbf{z}_k]. \quad (7)$$

If the variance of the measurement $\sigma_n^2$, is the same for all locations and readings, then the covariance matrix can be expressed as:

$$\mathbf{S} = \sigma_{\mathrm{n}}^2\mathbf{I}. \quad (8)$$

Thus:

$$L = \sigma_{\mathrm{n}}^{-2}\sum_{k=1}^{K}(\mathbf{\Phi}_k-\mathbf{z}_k)^{\mathrm{T}}(\mathbf{\Phi}_k-\mathbf{z}_k). \quad (9)$$

It can be seen that, under these restrictions on the noise of the measurements, the maximum likelihood approach reduces to the least squares approach.

In the above approach, the measurements $\mathbf{z}$ are considered to be in error because of experimental noise while the predicted responses are taken to be error free. In reality, the accuracy of the predicted responses depends upon the calculational procedure and the degree of approximation used, e.g. finite difference or finite element, coarse vs fine mesh, etc. These calculations give rise to errors (termed type 1 errors) in the predictions. In addition to these errors, the predictions will also exhibit variations,† which are due to the uncertainties in the parameters used in the calculations (referred to as type 2 errors). Of these two kinds of errors, type 1 errors can be mitigated by an astute choice of the numerical method or grids [6]. The effect of the type 2 errors on the predictions can be considerable and there are no known techniques to predict or to reduce these effects. An example of the effect of type 2 errors can be found in ref. [7], where variations in surface emissivity and thermal conductivities had a strong influence on the predicted temperatures of a thermal protection system used in re-entry vehicles. Presuming that type 1 errors have been eliminated, the estimated values of the parameters will be influenced by the type 2 errors. Therefore, there is a need to develop a technique which will compensate for the type 2 errors in the inverse problem solution and will reduce the effect of these uncertainties on the estimated parameters.

A logical approach to account for the type 2 errors in the numerical prediction is to consider the differences between the predictions and the measurements. Let the residual be given as:

$$\mathbf{\Psi}_k = \mathbf{\Phi}_k - \mathbf{z}_k, \quad (10)$$

where $\mathbf{\Phi}_k$, $\mathbf{z}_k$, and thus $\mathbf{\Psi}_k$, are assumed to be normally distributed and $\mathbf{\Phi}_k$ and $\mathbf{z}_k$ are assumed to be independent of each other. Since, by definition, $E[\mathbf{\Phi}_k] = E[\mathbf{z}_k]$, the mean of $\mathbf{\Psi}_k$ will be:

$$E[\mathbf{\Psi}_k] = 0, \quad (11)$$

and the covariance matrix $\mathbf{V}_k$ is given as:

$$\mathbf{V}_k = E[\{\mathbf{\Psi}_k - E[\mathbf{\Psi}_k]\}\{\mathbf{\Psi}_k - E[\mathbf{\Psi}_k]\}^{\mathrm{T}}] = E[\delta\mathbf{\Phi}_k\,\delta\mathbf{\Phi}_k^{\mathrm{T}}] + E[\delta\mathbf{z}_k\,\delta\mathbf{z}_k^{\mathrm{T}}], \quad (12)$$

where $\delta\mathbf{\Phi}_k = \mathbf{\Phi}_k - E[\mathbf{\Phi}_k]$. Because $\mathbf{\Psi}$ is normally distributed, the probability density function for $\mathbf{\Psi}$ can be given as:

$$f(\mathbf{\Psi}|\mathbf{u}) = \left[(2\pi)^{NK}\prod_{k=1}^{K} Det\,(\mathbf{V}_k)\right]^{-1/2} \times \exp\left[\sum_{k=1}^{K} -\tfrac{1}{2}\mathbf{\Psi}_k(\mathbf{u})^{\mathrm{T}}\mathbf{V}_k^{-1}\mathbf{\Psi}_k(\mathbf{u})\right]. \quad (13)$$

The criterion for estimation of the parameters, for this case, will then reduce to maximizing $J$, where $J$ is given as:

$$J = -2\ln f(\mathbf{\Psi}|\mathbf{u}) = \sum_{k=1}^{K}\ln\,[Det\,(\mathbf{V}_k)] + \sum_{k=1}^{K}\mathbf{\Psi}_k(\mathbf{u})^{\mathrm{T}}\mathbf{V}_k^{-1}\mathbf{\Psi}_k(\mathbf{u}). \quad (14)$$

In the above formulation, the covariance matrix $\mathbf{V}_k$, equation (12), consists of two parts, the covariance of $\mathbf{z}_k$ due to the experimental noise and the covariance

†Although these variations are not, strictly speaking, errors, we will refer to them as errors in subsequent sections.

of $\Phi_k$ due to the statistical nature of the known model parameters **b**. These known model parameters can be the physical properties, e.g. conductivity, heat capacity, etc. or they can be parameters defined on the boundaries, e.g. heat transfer coefficients, emissivity, etc. The information about these parameters is usually obtained from prior estimates in terms of their mean values $E[\mathbf{b}]$ and covariances **G**. The covariance matrix **G** represents the uncertainties in the known parameters **b** (i.e. the diagonal terms) and the correlation between the parameters (i.e. the non-diagonal terms). Thus **G** permits the use of the knowledge of parameters which are inter-related through a common cause, e.g. heat and mass transfer coefficients. An extensive discussion of the effects of these uncertainties on the system response can be found in ref. [8]. It can be shown [8] that the first-order estimate of the covariance matrix $E[\delta\Phi_k\delta\Phi_k^T]$ of the predictions is given by:

$$E[\delta\Phi_k\delta\Phi_k^T] = \Theta_k\mathbf{G}\Theta_k^T \quad k = 1,2,\ldots,K, \tag{15a}$$

where $\Theta_k$ is the sensitivity matrix defined as:

$$(\Theta_k)_{il} = \frac{\partial\phi(x_i,y_i,t_k)}{\partial B_l}$$

$$i = 1,2,\ldots,N \quad l = 1,2,\ldots,P \quad k = 1,2,\ldots,K, \tag{15b}$$

while the covariance matrix $E[\delta\mathbf{z}_k\delta\mathbf{z}_k^T]$ is calculated using equation (5). Therefore equation (12) can be expressed as:

$$\mathbf{V}_k = \Theta_k\mathbf{G}\Theta_k^T + \mathbf{S}_k. \tag{16}$$

The advantage of using the $J$ functional in place of the $L$ functional will be demonstrated for the following example.

## EXAMPLE—THE ESTIMATION OF THERMAL CONDUCTIVITY

Consider a slab of thickness $l$ (= 0.04 m) with an initial temperature of 0°C with a convective heat transfer boundary condition on both the back ($x = 0$) and the front ($x = l$) surfaces. The plate has a conductivity $k = 1.0$ W m$^{-1}$ °C$^{-1}$ and volumetric heat capacity $\rho c = 1.0\times10^6$ J m$^{-3}$ °C$^{-1}$. The plate is convectively heated with an ambient temperature of $T_\infty = 1000$°C on both the sides but with different heat transfer coefficients ($h_b = 5$ W m$^{-2}$ °C$^{-1}$ on the back surface and $h_f = 20$ W m$^{-2}$ °C$^{-1}$ on the front surface). The steady-state temperature distribution, being spatially constant, cannot be used to determine the thermal diffusivity of the plate or the heat transfer coefficients on the boundaries. On the other hand, the transient temperatures of the plate depend upon the thermal properties of the plate and the convective boundary conditions, and so can be used to estimate these parameters.

Let the conductivity $k$ of the plate be an unknown parameter which will be estimated by comparing experimentally measured temperatures with predicted temperatures. These experimentally measured temperatures are simulated by adding numerical noise to the solution of the direct problem with $k = 1$. This experimental noise is derived from a normally distributed random number with zero mean. Because the accuracy of the estimated parameters is not linear with respect to the noise in the measured temperatures, two levels of noise were considered for this example, a low noise ($\delta_n = 1\%$) and a high noise ($\delta_n = 5\%$). The standard deviation of the measured temperatures, $\sigma_n$, is given by:

$$\sigma_n^2 = \frac{\sum_{k=1}^{K}\sum_{i=1}^{N}(\delta_n\phi(x_i,y_i,t_k)\mathrm{N}[0,1])^2}{KN-1}, \tag{17}$$

where N[0, 1] is the normally distributed random number with zero mean and a standard deviation of unity.

The predicted temperatures require the specification of the heat transfer coefficients, which in a real experiment are not known exactly. One approach (the Monte Carlo method) is to assume a reasonable range of values for the coefficients and to repeat the calculations for a great number of values sampled from this range. Because the standard maximum likelihood approach does not account for uncertainty in the 'known' parameters (the convective heat transfer coefficients in this example) this sampling technique is the only approach possible. The method which we are presenting in this paper is designed to permit one to account for the uncertainty in the heat transfer coefficients by specifying a mean value and a standard deviation of the heat transfer coefficient.

In order to compare these two approaches, let us consider that the estimate of the heat transfer coefficient on the front surface of the slab $h_f$ is not accurate and that its value is distributed about the mean value $h_f$ with a standard deviation of $\sigma_h$. This can be expressed similarly to the temperature noise as $\sigma_h^2 = (\delta_h h_f)^2$. Again, because of the nonlinear nature of the relations, two levels of uncertainties in the heat transfer coefficient were considered, viz. $\delta_h = 10\%$ and $\delta_h = 30\%$. For this problem, since there is only one parameter to be estimated ($P = 1$), $\mathbf{u} = k$, and one parameter with uncertainty ($Q = 1$), $\mathbf{b} = h_f$, the covariances matrices **G**, $\mathbf{S}_k$, and $\mathbf{V}_k$ reduce to scalars with $\mathbf{G} = \sigma_h^2, \mathbf{S} = \sigma_n^2$, $\Theta_k$ is found by differentiating the closed form analytical solution to the temperature, and $V_k$ is found from equation (16).

*Numerical search method*

The estimated value of the conductivity is that which minimizes the functionals $L$ [equation (9)] and $J$ [equation (14)]. There are several numerical techniques which can be used to determine this minimum point of nonlinear functionals, ranging from the simple direct search method to complex variants of the Newton–Raphson method. In this section, we wish to

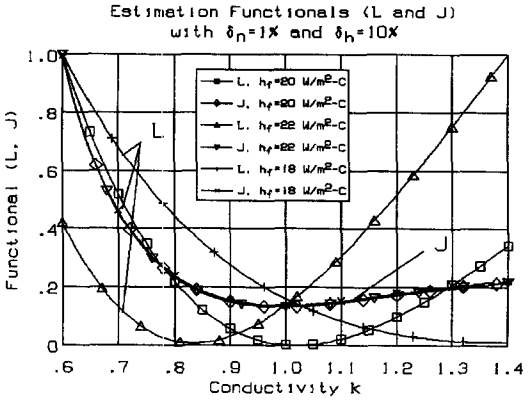


Fig. 1. Comparison of functional $J$ with functional $L$.

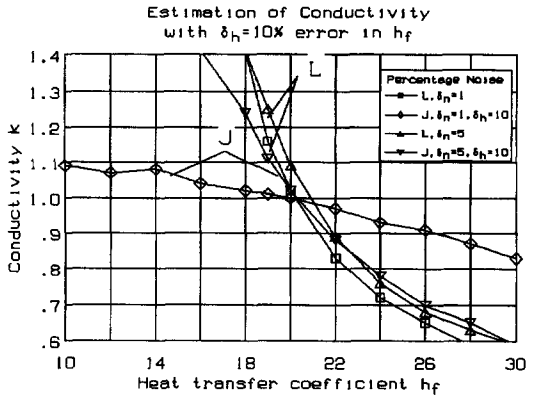


Fig. 2. Effect of 10% uncertainty in the heat transfer coefficient on the estimated conductivity.

demonstrate the superiority of the $J$ functional to the $L$ functional, without introducing the effects of the minimization technique. For this reason we have chosen a single parameter problem (e.g. the estimation only of $k$) with a single model parameter uncertainty ($h_f$) to which the straightforward direct search method can be applied.

Figure 1 displays the behavior of these two functionals based upon 10 equally spaced readings in time ($K = 10$), of the experimental measurements at $x = 0$ ($N = 1$). The values of $L$ and $J$ are dependent upon the convective heat transfer coefficient assumed in the calculation. Three cases were considered: (a) when the mean value of the heat transfer coefficient, $h_f$, used in the calculation was exact ($h_f = 20$); (b) when it was overestimated by 10% ($h_f = 22$); and (c) when it was underestimated by 10% ($h_f = 18$). In all three cases the uncertainty in $h_f$ was 10% (i.e. $\delta_h = 10\%$). It was observed that, for the first case when $h_f$ was exact, both approaches correctly estimate the conductivity to be $k = 1$ W m$^{-1}$ °C$^{-1}$, as expected, but the curve for $J$ was much shallower and the minimum value is harder to locate. For cases (b) and (c) minimizing $L$ gave an 18% and 38% error in the estimated conductivity, respectively. On the other hand minimizing $J$ gave rise to an error of less than 2% in the estimated conductivity for both cases.

The effect of a wide range of assumed heat transfer coefficient ($h_f = 10$–$30$) and the noise is illustrated in Fig. 2, where it is seen that $L$ is extremely sensitive to the assumed value of $h_f$ and even a slight error in $h_f$ leads to significant errors in the estimated value of $k$. When the noise level in the measured temperatures is low compared to the uncertainty in $h_f$ ($\delta_n = 1\%$, $\delta_h = 10\%$) the functional $J$ is very stable in estimating $k$. On the other hand, when the noise level is relatively high ($\delta_n = 5\%$, $\delta_h = 10\%$) $J$ is no better than $L$. The effect of the uncertainty in $h_f$ is further demonstrated in Fig. 3, where $\delta_h = 30\%$ for the two levels of noise. In this case, $J$ performs well for both noise levels.

The use of two sensors was also studied. The second sensor was placed at $x = l$ ($N = 2$). Again the performance of the $J$ criterion was better than that of the

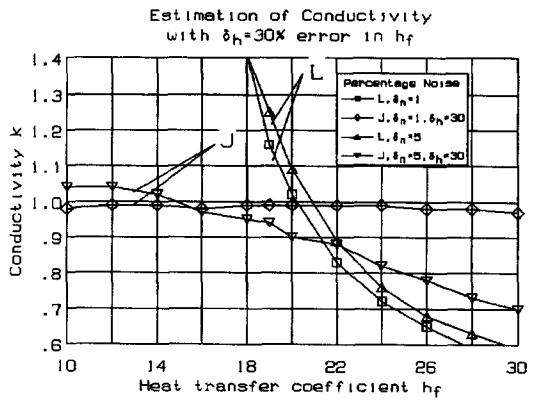


Fig. 3. Effect of 30% uncertainty in the heat transfer coefficient on the estimated conductivity.

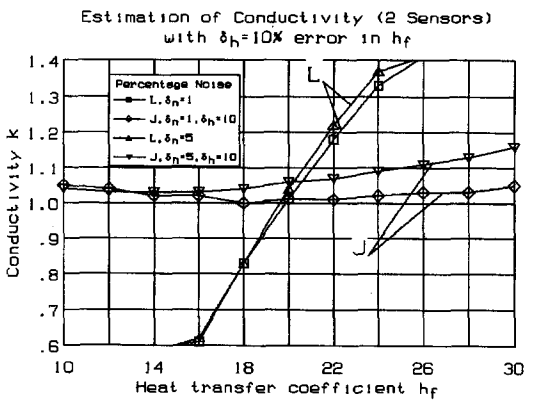


Fig. 4. Effect of 10% uncertainty in the heat transfer coefficient on the estimated conductivity for two sensors.

$L$ criterion. Figure 4 shows the performance of both criteria for $\delta_h = 10\%$. The $L$ criterion is unimproved by the addition of the second sensor. However, for the $J$ criterion, the second sensor substantially decreases the deleterious effect of noise on the estimation of the conductivity (compare the curves for $J$ in Figs. 2 and 4).

*Newton–Raphson method*

The minimization of the likelihood functional defined by equation (14) is a unconstrained nonlinear problem of optimization. In the example given, since only the conductivity is unknown and only one parameter has uncertainty, it is possible to use a direct search procedure to find the minimum point. In general, several parameters are sought and a multidimensional procedure is needed. Let $\mathbf{u}^n$ be the estimated unknown parameters after the $n$ iterations. Then the estimate after $n+1$ iterations is given by $\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta\mathbf{u}^{n+1}$. The functional at the $n+1$ iteration is $J(\mathbf{u}^{n+1}) = J(\mathbf{u}^n + \Delta\mathbf{u}^{n+1})$. Expressing this in a Taylor series expansion gives:

$$J(\mathbf{u}^n+\Delta\mathbf{u}^{n+1}) = J(\mathbf{u}^n) + [\mathbf{J}'(\mathbf{u}^n)]^{\mathrm{T}}\Delta\mathbf{u}^{n+1} + \tfrac{1}{2}(\Delta\mathbf{u}^{n+1})^{\mathrm{T}}\mathbf{J}''(\mathbf{u}^n)\Delta\mathbf{u}^{n+1} + O(\|\Delta\mathbf{u}^{n+1}\|^3), \quad (18)$$

where:

$$[\mathbf{J}'(\mathbf{u}^n)]_l = \frac{\partial J(\mathbf{u}^n)}{\partial u_l} \quad l = 1, 2, \ldots, P,$$

and:

$$[\mathbf{J}''(\mathbf{u}^n)]_{lm} = \frac{\partial^2 J(\mathbf{u}^n)}{\partial u_l \partial u_m} \quad l, m = 1, 2, \ldots, P.$$

The condition for minimization is therefore:

$$\left[\frac{\partial J(\mathbf{u}^n+\Delta\mathbf{u}^{n+1})}{\partial \mathbf{u}^{n+1}}\right] = \mathbf{J}'(\mathbf{u}^n) + \mathbf{J}''(\mathbf{u}^n)\Delta\mathbf{u}^{n+1} + O(\|\Delta\mathbf{u}^{n+1}\|^2) = 0, \quad (19)$$

and thus:

$$\mathbf{u}^{n+1} = \mathbf{u}^n - [\mathbf{J}''(\mathbf{u}^n)]^{-1}\mathbf{J}'(\mathbf{u}^n). \quad (20)$$

While deriving expressions for $\mathbf{J}'(\mathbf{u}^n)$ and $\mathbf{J}''(\mathbf{u}^n)$ use was made of the matrix identity:

$$\frac{\partial \ln [Det\,(\mathbf{V}_k)]}{\partial u_l} = Tr\left(\mathbf{V}_k^{-1}\frac{\partial \mathbf{V}_k}{\partial u_l}\right).$$

The proof of the above identity is given in the Appendix. Using this identity it can then be shown that:

$$\frac{\partial J}{\partial u_l} = \sum_{k=1}^{K}\left[Tr\left(\mathbf{V}_k^{-1}\frac{\partial \mathbf{V}_k}{\partial u_l}\right) + 2\left(\frac{\partial \mathbf{\Phi}_k}{\partial u_l}\right)^{\mathrm{T}}\mathbf{V}_k^{-1}(\mathbf{\Phi}_k - \mathbf{z}_k) - (\mathbf{\Phi}_k - \mathbf{z}_k)^{\mathrm{T}}\mathbf{V}_k^{-1}\frac{\partial \mathbf{V}_k}{\partial u_l}\mathbf{V}_k^{-1}(\mathbf{\Phi}_k - \mathbf{z}_k)\right], \quad (21a)$$

and:

$$\frac{\partial^2 J}{\partial u_l \partial u_m} = \sum_{k=1}^{K}\left[Tr\left(\mathbf{V}_k^{-1}\frac{\partial^2 \mathbf{V}_k}{\partial u_l \partial u_m}\right) - Tr\left(\mathbf{V}_k^{-1}\frac{\partial \mathbf{V}_k}{\partial u_m}\mathbf{V}_k^{-1}\frac{\partial \mathbf{V}_k}{\partial u_l}\right) + 2\left(\frac{\partial^2 \mathbf{\Phi}_k}{\partial u_l \partial u_m}\right)^{\mathrm{T}}\mathbf{V}_k^{-1}(\mathbf{\Phi}_k - \mathbf{z}_k) - 2\left(\frac{\partial \mathbf{\Phi}_k}{\partial u_l}\right)^{\mathrm{T}}\mathbf{V}_k^{-1}\frac{\partial \mathbf{V}_k}{\partial u_m}\mathbf{V}_k^{-1}(\mathbf{\Phi}_k - \mathbf{z}_k) + 2\left(\frac{\partial \mathbf{\Phi}_k}{\partial u_l}\right)^{\mathrm{T}}\mathbf{V}_k^{-1}\frac{\partial \mathbf{\Phi}_k}{\partial u_m} - 2\left(\frac{\partial \mathbf{\Phi}_k}{\partial u_m}\right)^{\mathrm{T}}\mathbf{V}_k^{-1}\frac{\partial \mathbf{V}_k}{\partial u_l}\mathbf{V}_k^{-1}(\mathbf{\Phi}_k - \mathbf{z}_k) + 2(\mathbf{\Phi}_k - \mathbf{z}_k)^{\mathrm{T}}\mathbf{V}_k^{-1}\frac{\partial \mathbf{V}_k}{\partial u_l}\mathbf{V}_k^{-1}(\mathbf{\Phi}_k - \mathbf{z}_k) - (\mathbf{\Phi}_k - \mathbf{z}_k)^{\mathrm{T}}\mathbf{V}_k^{-1}\frac{\partial^2 \mathbf{V}_k}{\partial u_l \partial u_m}\mathbf{V}_k^{-1}(\mathbf{\Phi}_k - \mathbf{z}_k)\right], \quad (21b)$$

where:

$$\frac{\partial \mathbf{V}_k}{\partial u_l} = 2\mathbf{\Theta}_k\mathbf{G}\frac{\partial \mathbf{\Theta}_k^{\mathrm{T}}}{\partial u_l} + \frac{\partial \mathbf{S}_k}{\partial u_l}, \quad (21c)$$

and:

$$\frac{\partial^2 \mathbf{V}_k}{\partial u_l \partial u_m} = 2\frac{\partial \mathbf{\Theta}_k}{\partial u_m}\mathbf{G}\frac{\partial \mathbf{\Theta}_k^{\mathrm{T}}}{\partial u_l} + 2\mathbf{\Theta}_k\mathbf{G}\frac{\partial^2 \mathbf{\Theta}_k^{\mathrm{T}}}{\partial u_l \partial u_m} + \frac{\partial^2 \mathbf{S}_k}{\partial u_l \partial u_m}. \quad (21d)$$

In evaluating $\mathbf{J}'$ and $\mathbf{J}''$, i.e. equations (21a)–(21d), it is necessary to determine the first- and second-order derivatives of $\mathbf{\Phi}$ and $\mathbf{\Theta}$ with respect to the unknown parameters $\mathbf{u}$. But $\mathbf{\Theta}$, the sensitivity matrix, consists of first-order derivatives of $\mathbf{\Phi}$ with respect to the known parameters $\mathbf{b}$, equation (15b). This leads to third-order derivatives of $\mathbf{\Phi}$. Hence evaluation of $\mathbf{J}'$ and $\mathbf{J}''$ is computationally expensive and the solution procedure for equation (20) should be as efficient as possible. There are three approaches to evaluating these higher-order derivatives of the temperature field from the field equations:

(a) simply differencing the results obtained from the solution of the field equations for $\mathbf{u}$ and $\mathbf{u}+\Delta\mathbf{u}$ [5]. This approach was used in the example presented in this paper;
(b) solve the differentiated field equations [9]; and
(c) using the adjoint method [10, 11].

In general, the technique for minimizing $J$ takes the form of an iterative procedure which leads to a sequence of estimates, which, if the method is successful, converges more or less rapidly. Convergence is usual if the functional to be minimized is strictly convex and parabolic, at least in the neighborhood of the minimum, and that the initial guess is in this region of convexity [12]. In the absence of prior knowledge of the behavior of the functional it is difficult to ensure this. This is a common problem in the use of Newton's approach to minimization/maximization. A modification to this approach was suggested by Goldfield *et al.* [13]. The modification uses a factor $\alpha$ in equation (20). This $\alpha$ is defined as:

$$\alpha = \lambda_{\mathrm{P}} + R\,\|\mathbf{J}'(\mathbf{u}^n)\| \quad (22)$$

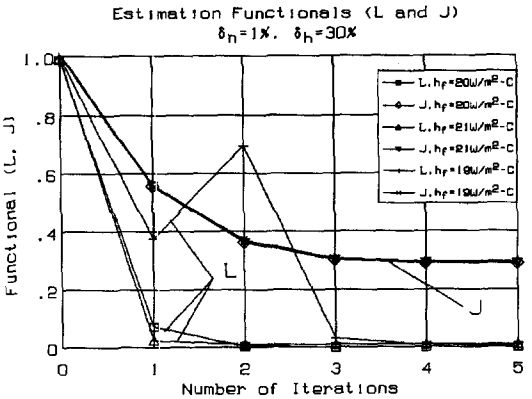


Fig. 5. Behavior of functionals during iterations.

where $\lambda_P$ is the smallest eigenvalue of $\mathbf{J}''(\mathbf{u}^n)$ and $R$ is a positive weight. The recursive relation for the $n+1$th estimate then reduces to:

$$\mathbf{u}^{n+1} = \mathbf{u}^n - [\mathbf{J}''(\mathbf{u}^n) + \beta \mathbf{I}]^{-1} \mathbf{J}'(\mathbf{u}^n)$$

$$\beta = \begin{cases} 0, & \text{for } \alpha > 0, \\ \alpha, & \text{for } \alpha \leqslant 0. \end{cases} \tag{23}$$

Finally, the convergence criterion used in this algorithm is:

$$\frac{\|\mathbf{u}^{n+1} - \mathbf{u}^n\|}{\|\mathbf{u}^n\|} \leqslant \varepsilon, \tag{24}$$

where $\varepsilon$ is the expected measure of accuracy. This algorithm, equation (23), was verified by comparing its results with those obtained by a direct search method.

Equations (20)–(23) were used to minimize $L$ [equation (9)] and $J$ [equation (14)] with a convergence criterion of $\varepsilon = 0.001$ and $R$ selected to be the reciprocal of the determinant of $\mathbf{J}''$. The rate of convergence is shown in Figs. 5 and 6. For both functionals the initial guess of the unknown parameter (conductivity) was taken to be 0.7, the noise level to be $\delta_n = 1\%$ and the uncertainty in the heat transfer coefficient to be $\delta_h = 30\%$. Figure 5 shows the rate of convergence for different values of $h_f$. Figure 6 shows the corresponding estimates of the conductivity $k$. Figure 5 shows that if the functional $L$ approaches the minimum monotonically then the functional quickly drops to the minimum, otherwise the approach is oscillatory. The functional $J$ always approaches smoothly and gradually. It can also be seen that the $h_f$ value has no effect on the convergence of $J$. These observations are also seen in Fig. 6 where the successive estimates of the conductivity are plotted against the number of iterations and the oscillatory approach of the functional $L$ is obvious.

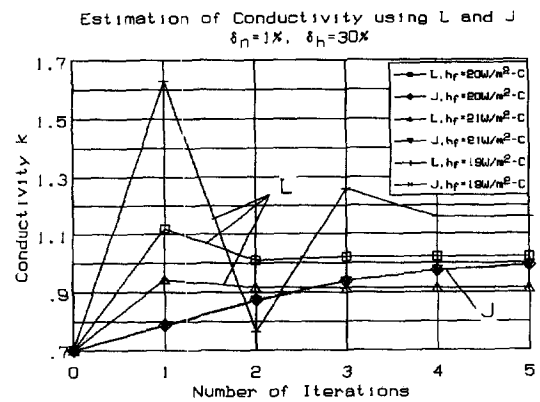


Fig. 6. Estimated conductivity during iterations.

## CONCLUSIONS

A new functional for parameter estimation is proposed which will not only account for the effects of the experimental noise on the estimated parameters but, in addition, will minimize the effects of the uncertainties in the assumed model parameters upon the parameters being sought. The development of this new functional was achieved through the synthesis of two well-known approaches, viz. the principle of maximum likelihood, popularly used in inverse problems with experimental noise, and the first-order, second moment approach used to study the effects of uncertainties in systems on the response of the system. Through the use of the example, it is demonstrated that, in the presence of uncertain model parameters, the proposed new functional is superior to the usual maximum likelihood approach. An efficient numerical algorithm for the minimization of the proposed functional has also been developed.

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## APPENDIX

*Matrix identities*

*Statement* I. Let $\mathbf{V}$ be a $N \times N$ real, positive definite, symmetric matrix such that each element of $\mathbf{V}$ is a real function of a scalar $u$. Let the eigenvalue of $\mathbf{V}$ be given by $\lambda$ and the corresponding eigenvector given by $\mathbf{q}$ such that $\mathbf{V}\mathbf{q} = \lambda\mathbf{q}$; then:

$$\left[\mathbf{V}^{-1}\frac{\partial \mathbf{V}}{\partial u}\right]\mathbf{q} = \lambda^{-1}\frac{\partial \lambda}{\partial u}\mathbf{q}. \tag{A1}$$

*Proof.* Since the eigenvectors are orthogonal:

$$\frac{\partial \mathbf{q}}{\partial u} = -\mathbf{q}\frac{\partial \mathbf{q}^{\mathrm{T}}}{\partial u}\mathbf{q}. \tag{A2}$$

Also, multiplying the characteristic equation by $\mathbf{V}^{-1}$ gives

$$\mathbf{V}^{-1}\mathbf{q} = \frac{1}{\lambda}\mathbf{q}. \tag{A3}$$

Now let

$$\frac{\partial \mathbf{q}^{\mathrm{T}}}{\partial u}\mathbf{q} = a, \tag{A4}$$

where $a$ is a scalar quantity.

Differentiating the characteristic equation and then multiplying it by $\mathbf{V}^{-1}$ gives:

$$\left[\mathbf{V}^{-1}\frac{\partial \mathbf{V}}{\partial u} - \frac{\partial \lambda}{\partial u}\mathbf{V}^{-1}\right]\mathbf{q} = [\lambda\mathbf{V}^{-1} - \mathbf{I}]\frac{\partial \mathbf{q}}{\partial u}. \tag{A5}$$

Substituting equations (A2), (A3) and (A4) in equation (A5) will give:

$$\left[\mathbf{V}^{-1}\frac{\partial \mathbf{V}}{\partial u} - \frac{1}{\lambda}\frac{\partial \lambda}{\partial u}\mathbf{I}\right]\mathbf{q} = -a\lambda\left[\mathbf{V}^{-1} - \frac{1}{\lambda}\mathbf{I}\right]\mathbf{q} \equiv 0. \tag{A6}$$

Therefore, $\lambda^{-1}\,\partial\lambda/\partial u$ is the eigenvalue of the matrix $\mathbf{V}^{-1}\,\partial\mathbf{V}/\partial u$ and proves statement I.

*Statement* II. Let $\mathbf{V}$ be an $N \times N$ real positive definite symmetric matrix such that each element of $\mathbf{V}$ is a real function of a scalar $u$; then:

$$\frac{\partial \ln [Det\,(\mathbf{V})]}{\partial u} = Tr\left(\mathbf{V}^{-1}\frac{\partial \mathbf{V}}{\partial u}\right). \tag{A7}$$

Proof. Let $\lambda_1, \lambda_2, \ldots, \lambda_N$ be the eigenvalues of the matrix $\mathbf{V}$. Since matrix $\mathbf{V}$ is real and symmetric, all its eigenvalues are real numbers and all its eigenvectors are orthogonal. The matrix $\mathbf{V}$ can then be expressed as:

$$\mathbf{V}\mathbf{Q} = \mathbf{Q}\mathbf{\Lambda} \quad \text{or} \quad \mathbf{V} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^{\mathrm{T}}, \tag{A8}$$

where $\mathbf{Q}$ is the orthogonal matrix of eigenvectors and $\mathbf{\Lambda}$ is the diagonal matrix of eigenvalues. Therefore the determinant of the matrix $\mathbf{V}$ will be given as:

$$Det\,(\mathbf{V}) = Det\,(\mathbf{Q})\,Det\,(\mathbf{\Lambda})\,Det\,(\mathbf{Q}^{\mathrm{T}}) = \prod_{i=1}^{N}\lambda_i. \tag{A9}$$

Taking the derivative of the logarithm of the determinant leads to:

$$\frac{\partial}{\partial u}\left(\ln\prod_{i=1}^{N}\lambda_i\right) = \sum_{i=1}^{N}\lambda_i^{-1}\frac{\partial \lambda_i}{\partial u}. \tag{A10}$$

It can be shown that, for any matrix with distinct eigenvalues, the sum of all its eigenvalues is also equal to the sum of its diagonal terms. The proof of this theorem can be found in Graybill [14] (Therorem 9.1.3, p. 299). Making use of this theorem and using Statement I, gives:

$$\sum_{i=1}^{N}\lambda_i^{-1}\frac{\partial \lambda_i}{\partial u} = Tr\left[\mathbf{V}^{-1}\frac{\partial \mathbf{V}}{\partial u}\right]. \tag{A11}$$

This proves statement II.