# Optimal Regularization of the Inverse Heat-Conduction Problem

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**The solution of the inverse heat conduction problem is obtained using dynamic programming and generalized cross-validation to estimate the optimal regularization parameter. Generalized cross-validation is appealing because it uses only the data to estimate the optimal value of the regularization parameter. The calculations for generalized cross-validation are performed as an extension of dynamic programming. A discussion of the problem and a brief outline of the computational steps are given. Several numerical examples are included to demonstrate the validity and limitations of the method.**

## Nomenclature

$A$ = global influence matrix, see Eq. (20)
$A_{ij}$ = submatrix of $A$ $(n_z \times n_z)$
$b$ = regularization parameter
$B$ = diagonal matrix $(b)$, $(n_q \times n_q)$
$c$ = specific heat
$C$ = capacitance matrix $(n \times n)$
$d_j$ = measurements at step $j(n_z \times 1)$
$D$ = intermediate matrix $(n_q \times n_q)$, see Eq. (8)
$E$ = intermediate matrix $(n \times n)$, see Eq. (11)
$E_N$ = least-squares error, see Eq. (7)
$h$ = integration time step
$H$ = intermediate matrix $(n_q \times n)$, see Eq. (9)
$I$ = identity matrix $(n \times n)$
$k_x, k_y$ = thermal conductivity
$K$ = conductance matrix $(n \times n)$
$M$ = transformation matrix $(n \times n)$, see Eq. (3)
$\hat{M}$ = intermediate matrix $(n \times n)$, see Eq. (10)
$n$ = number of temperatures
$n_q$ = number of unknown heat fluxes
$n_Z$ = number of measurements
$N$ = total number of time steps
$P$ = influence matrix $(n \times n_q)$, see Eq. (3)
$q$ = unknown heat fluxes $(n_q \times 1)$
$q_k$ = estimated heat flux $(n_q \times 1)$
$\hat{q}$ = true heat flux $(n_q \times 1)$
$Q$ = heat-flux participation matrix $(n \times n_q)$, see Eq. (1)
$r$ = heat-flux derivative $(n_q \times 1)$
$R$ = Riccati matrix $(n \times n)$
$S$ = true least-squares error for heat flux, see Eq. (18)
$S$ = recursive vector $(n \times 1)$, see Eq. (13)
$T$ = temperature
$T$ = unknown temperatures $(n \times 1)$
$U$ = measurement matrix $(n_z \times n)$, see Eq. (6)
$V$ = generalized cross-validation function, see Eq. (19)
$W$ = generalized cross-validation matrix $(n \times n)$, see Eq. (21)
$z_j$ = measured temperatures $(n_z \times 1)$, see Eq. (6)
$\rho$ = density

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## Introduction

THE inverse heat-conduction problem is concerned with the estimation of unknown heat fluxes based on measured temperature data. Although there have been many approaches to this problem (see Ref. 1), some of the most promising are the regulatization methods. These methods involve adding a term to the minimization problem to smooth and stabilize the solutions. The relative magnitude of this additional term is adjusted with the use of a regularization parameter. Until now there has not been a general technique for selecting regularization parameters.

Herein, the method of generalized cross-validation (GCV) will be used to estimate the optimal value of the regularization parameter.[2] GCV is appealing because it uses only the data to estimate the optimal value of the regularization parameter. Murio[10] discusses how the parameter may be selected if the noise level in the data is known. GCV has been used for splines,[3,4] and, recently, Dohrmann et al.[5] showed that the calculations for GCV could be performed as an extension of the dynamic programming formulas. Dynamic programming has been applied to the inverse heat-conduction problem.[6-8] A discussion of the problem and a brief outline of the computational steps are given. The results of numerical examples that demonstrate the validity and limitations of the GCV method are presented.

## Inverse Heat-Conduction Problem

The governing partial differential equation for the temperature within a region is

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right)$$

The physical parameters $\rho c$, $k_x$, and $k_y$ can vary spatially within the region. The boundary conditions considered in this problem involve imposed heat fluxes along the boundaries. Regardless of the shape of the region or whether a finite-difference or finite-element representation is used, the resulting model can be expressed as the following vector-matrix differential equation with corresponding initial conditions:

$$C\dot{T} = KT + Qq \tag{1}$$

$$T(0) = T_0 \tag{2}$$

where $K$ is an $(n \times n)$ conduction matrix, $C$ a diagonal capacitance matrix, $Q$ an $(n \times n_q)$ matrix, $q$ an $(n_q \times 1)$ vector representing the unknown forcing terms (heat fluxes), $T$ is an $(n \times 1)$ vector representing the unknown temperatures, and $\dot{T}$ represents the time derivative.

The inverse problem we are concerned with is one in which the system matrices $K$ and $C$ are known, together with information on some or all of the temperature variables; however, the forcing term $q$ is unknown. Thus, the problem can be stated as follows: Given the system matrices $K$ and $C$ and measurements of temperatures, find the forcing term $q$ that causes the system [Eq. (1)] to best match the measurement.

The differential equation (1) can be integrated with a number of equivalent discrete-time models, including the Crank-Nicolson or Padé formulas. Regardless of which formula is used, the result is a difference equation of the form

$$T_{j+1} + MT_j + Pq_j \tag{3}$$

In this study, the exponential matrix representation was used. Thus, $M$ is the exponential matrix of matrix $K$ for an integration step side $h$:

$$M = e^{C^{-1}Kh} \tag{4}$$

$$P = K^{-1}(M - I)Q \tag{5}$$

The mathematical representation of the concept mentioned earlier—"best match the measurement"—will be a least-squares criterion. In most cases, it is not possible to measure all of the variables $T_j$, and, in some cases, only certain combinations of the variables are measured. A convenient expression that relates the model variables $T_j$ to the corresponding measurements $d_j$ is

$$z_j = UT_j \tag{6}$$

where $z_j$ is an $n_z \times 1$ vector and $U$ is an $n_z \times n$ matrix. The measurements are represented by a vector $d_j$ of the same dimension as $z_j$.

The least-squares error is now expressed as

$$E_N(T_0, q_j) = \sum_{j=1}^{N} [z_j - d_j, (z_j - d_j)] + b(q_j, q_j) \tag{7}$$

where $(x,y)$ denotes the inner product of two vectors. The scalar $b$ is called the "regularization parameter." The inverse solution is to find the fluxes $q_j$ that minimize Eq. (7) while satisfying Eq. (3).

The inclusion of $(q_j, q_j)$ will play a crucial part in the solution to the inverse problem. The reason it is included as part of the error expression is to allow control of the behavior (smoothness) of the unknown forcing terms $q_j$. A small value of $b$ causes the solution to match the data closely but produces large oscillatory fluxes. A large value of $b$ produces smooth fluxes but may not match the data well. Thus, it is assumed that there is an optimal value of $b$ that produces a solution close to the true temperatures and heat fluxes.

## Dynamic Programming Recursive Formulas

The recursive formulas for the dynamic programming solution start at the endpoint of the data and constitute a backward sweep from $k = N$ to 1, followed by a forward sweep. The computations for a typical backward step from $k+1$ to $k$ are given next.

Intermediate variables:

$$D = (2B + 2P^T R_{k+1} P)^{-1} \tag{8}$$

$$H^T = 2R_{k+1}P \tag{9}$$

$$\hat{M}^T_{k+1} = M^T(I - H^T D P^T) \tag{10}$$

$$E_{k+1} = -PDP^T \tag{11}$$

The $R$ matrices and $S$ vectors are then computed using

$$R_k = U^T U + M^T(R_{k+1} - \tfrac{1}{2} H^T D H)M \tag{12}$$

$$S_k = -2U^T d_k + \hat{M}^T_{k+1} S_{k+1} \tag{13}$$

$B$ is a diagonal matrix containing the regularization parameter $b$ along the diagonal. The initial conditions for $R_N$ and $S_N$ are known at the end $(k = N)$ and are

$$R_N = U^T U \tag{14}$$

$$S_N = -2U^T d_N \tag{15}$$

Having computed all of $R_k$ and $S_k$, the second step is a forward sweep from $k = 1$ to $N$, which produces the final estimates for the temperatures and the heat fluxes.

$$q_k = -(2B + 2P^T R_{k+1} P)^{-1} P^T (S_{k+1} + 2R_{k+1} M T_k) \tag{16}$$

$$T_{k+1} = MT_k + Pq_k \tag{17}$$

## Generalized Cross-Validation

The basic idea of cross-validation is to use the data to estimate the true mean-square error. (See the discussion by Woltring.[4]) This is done for a fixed $b$ by deleting one of the data points in the inverse solution. The resulting solution is then used to predict the value of the missing data point. Using this predicted value and the missing data point provides an error estimate for the data point. Repeating this for another data point provides another error estimate. If all of the data points are summed in a least-squares sense, then a total estimated error of predicted missing data is achieved. The value of $b$ that minimizes such an error should be very close to the optimal value.

In this paper, the optimal value of the regularization parameter is defined as one that causes the estimated $q_i$ to match best the true heat flux $\hat{q}_i$.

$$S(b) = \left[ \frac{1}{N} \sum_{i=1}^{N} (q_i - \hat{q}_i)^2 \right]^{1/2} \tag{18}$$

The "optimal $b^*$" is the one that minimizes Eq. (18).

Of course, in a real problem $S(b)$ cannot be computed since $\hat{q}_i$ is unknown. Neither the true temperatures nor the noise levels on the data are known. This is where the method of GCV enters. It provides a function, $V(b)$, that is calculated easily using only the data itself; no other information is necessary, because minimizing $V(b)$ is essentially the same as minimizing $S(b)$. The numerical experiments will demonstrate the validity and limitations of the methods.

## Generalized Cross-Validation Formulas

The formula for $V(b)$ is

$$V(b) = \left[ \frac{1}{N} \sum_{j=1}^{N} (z_j - d_j, z_j - d_j) \right] \Big/ \{(1/N)\ \mathrm{tr}[I - A(b)]\}^2 \tag{19}$$

where tr denotes the trace (sum of the diagonals) of a matrix. The matrix $A$ is a global matrix that relates all of the measurements to the estimated temperatures. That is,

$$\begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_N \end{bmatrix} = \begin{bmatrix} A_{11} A_{12} \cdots & & \\ A_{21} A_{22} \cdots & & \\ \vdots & & \vdots \\ & & A_{NN} \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_N \end{bmatrix} \tag{20}$$

The diagonal submatrices $A_{kk}$ are computed using the following recursive formula for a matrix $W_{kk}$:

$$W_{k+1,k+1} = \hat{M}_{k+1} W_{kk} \hat{M}^T_{k+1} - 2E_{k+1} \tag{21}$$

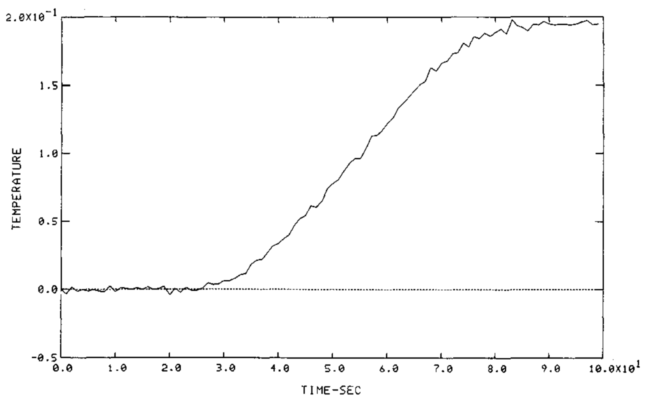


Fig. 1 Temperature data for example 1 ($\sigma = 0.002$).

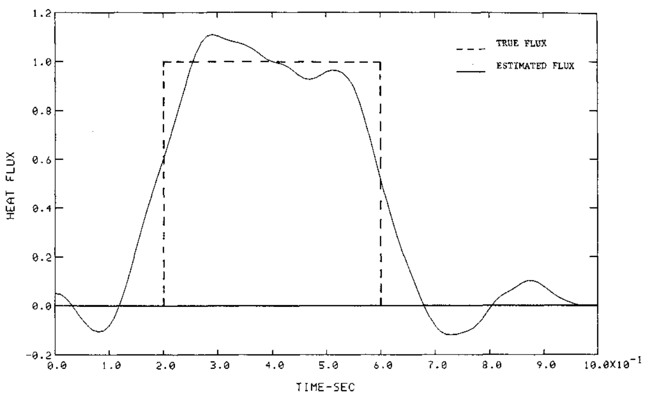


Fig. 3 Example 1 heat flux, $b = 1.72E-5$.

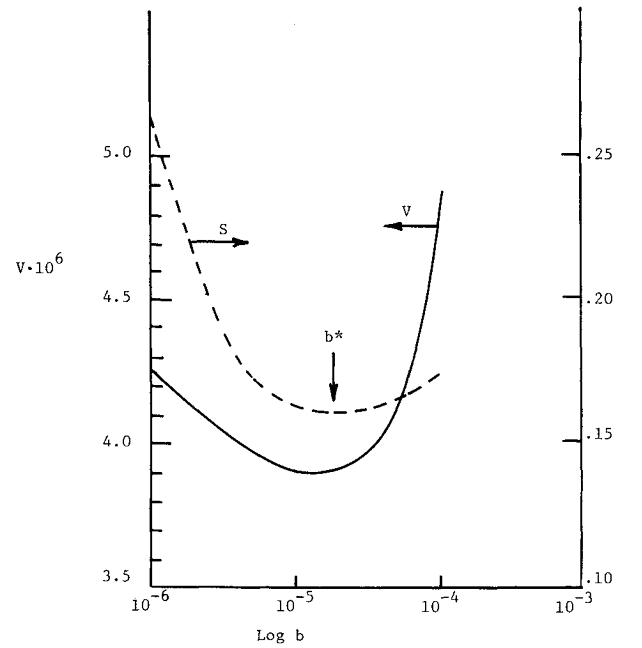


Fig. 2 Example 1—variation of $S$ and $V$ with the parameter $b$ ($\sigma = 0.002$).

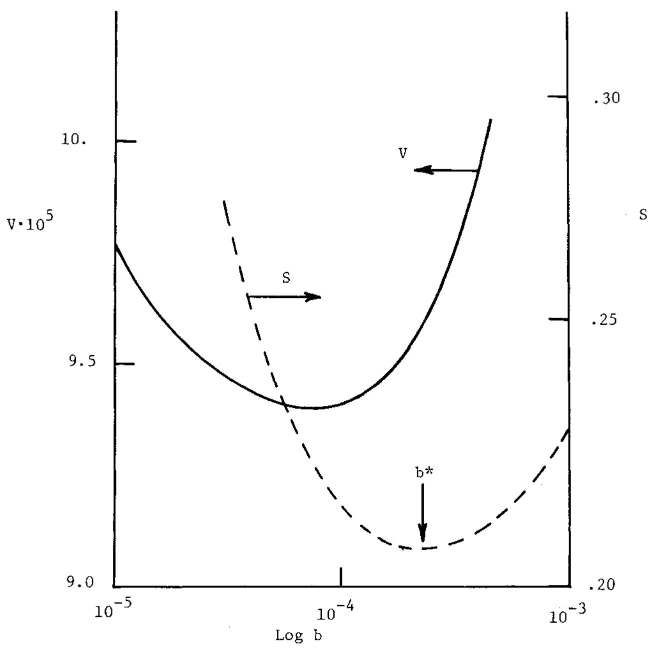


Fig. 4 Example 1—variation of $S$ and $V$ with the parameter $b$ ($\sigma = 0.010$).

The submatrix $A_{kk}$ is then computed using

$$A_{kk} = UW_{kk}U^T \tag{22}$$

If the initial temperatures are unknown, then the initial condition for $W_{11}$ is $R_1^{-1}$. For known initial temperatures, the formulas start at $W_{22} = -2E_{22}$.

The overall solution now involves two minimizations. The outer minimization is performed over $b$ by minimizing $V(b)$. For each value of $b$, the dynamic programming method is used to find the heat fluxes that minimize Eq. (7).

## Numerical Example 1

The first problem represents a semi-infinite slab subjected to a surface heat flux. This problem was analyzed in Ref. 9 using a different method of solution. The true heat flux is a unit flux between 0.2 and 0.6 s. For this example, a finite-difference model was constructed using a total of 41 nodes spaced a distance of 0.10 units and using unit properties. A time increment of 0.01 unit was used. The measurement is located at a distance of 1.0 units from the surface.

First, a random noise level of $\sigma = 0.002$ was added to the temperature. The resulting noisy data are shown in Fig. 1. Next, a series of inverse problems was solved varying only the regularization parameter, $b$. For each solution, the functions $S(b)$ and $V(b)$ were computed. The results are shown in Fig. 2, which illustrates the usefulness of the GCV method. Since the true heat flux is known, one would select $b$ to minimize $S(b)$. However, in a real situation, one can minimize only $V(b)$. Figure 2 illustrates the fact that the minimum of $V(b)$ gives an excellent estimate to the optimal regularization parameter, $b^*$. The heat flux obtained by using $b^*$ ($1.72E-5$) in the inverse solution is shown in Fig. 3.

This experiment was repeated for a larger noise level of $\sigma = 0.010$. Figure 4 shows the results. In this case, $V(b)$ does not yield the same minimum $b$ as $S(b)$ although they are in the same range. In addition, this noise level is fairly large, as illustrated in Fig. 5.

## Numerical Example 2

The second example is taken from Ref. 7 and represents a two-dimensional finite-element model involving *two* unknown heat fluxes and two temperature measurements. The finite-element model consisted 25 nodes and 16 quadrilateral elements. Unit properties were used. The heat fluxes were applied to two adjacent sides, with the other sides insulated. The measurements were located at the midpoints of the insulated sides. A time increment of 0.10 units was used. A noise level of 0.5 deg was added to the measurements, which varied from 0 to 336 deg.

Again a series of inverse problems was solved varying only the parameter $b$. Figure 6 shows the functions $V(b)$ and $S(b)$. $S(b)$ is computed using both heat fluxes. In this case, the optimal $b$ is not found by minimizing $V(b)$. If one were to use

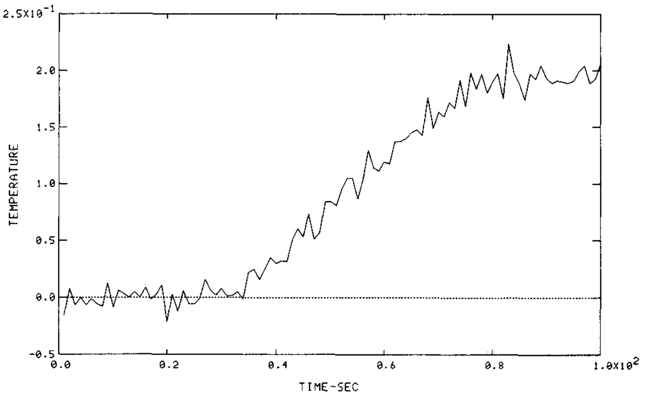


Fig. 5 Example 1 temperature data ($\sigma = 0.010$).

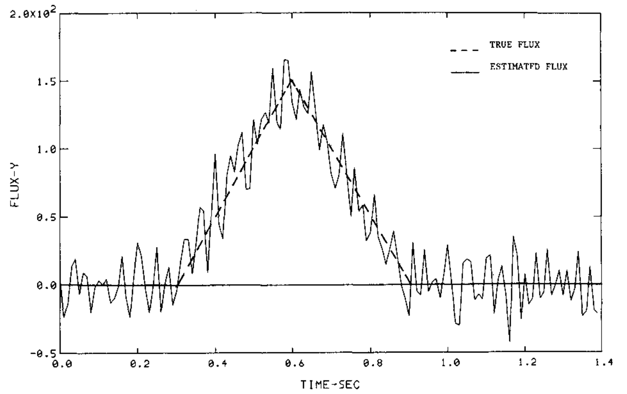


Fig. 8 Heat flux 2 for example 2 ($b = 8.79E - 5$).

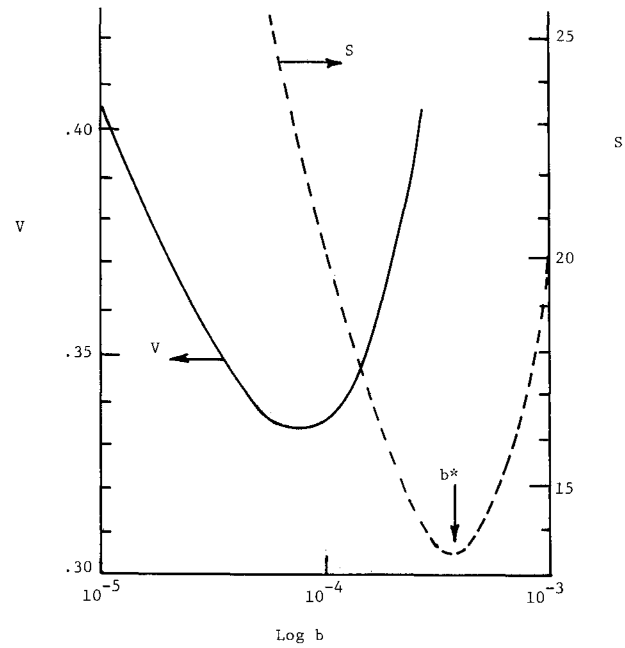


Fig. 6 Example 2—variation of $S$ and $V$ with parameter $b$.

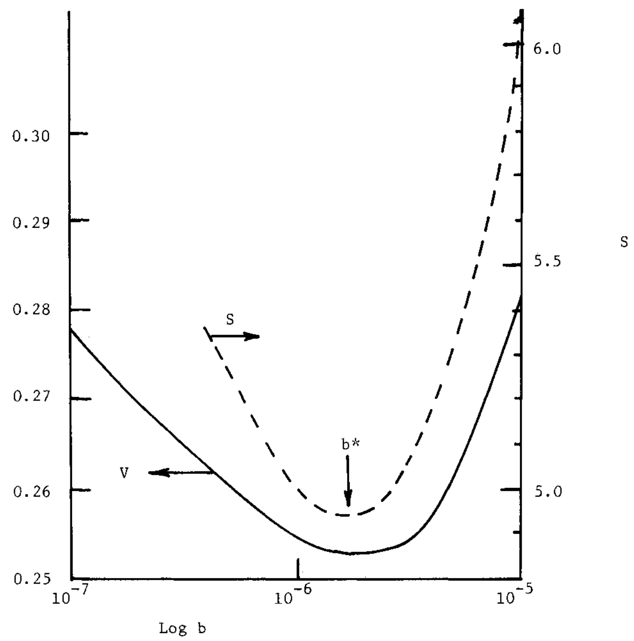


Fig. 9 Example 2—first-order regularization; variation of $S$ and $V$ with $b$.

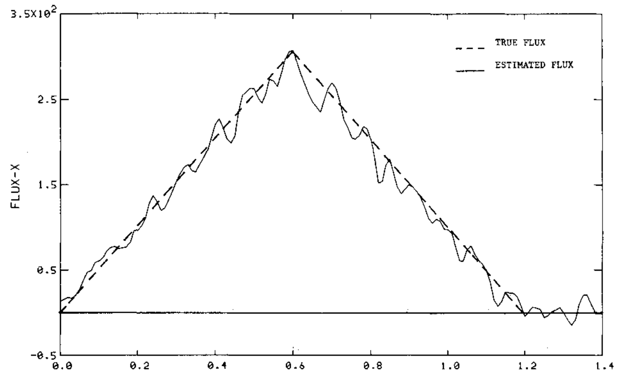


Fig. 7 Heat flux 1 for example 2 ($b = 8.79E - 5$).

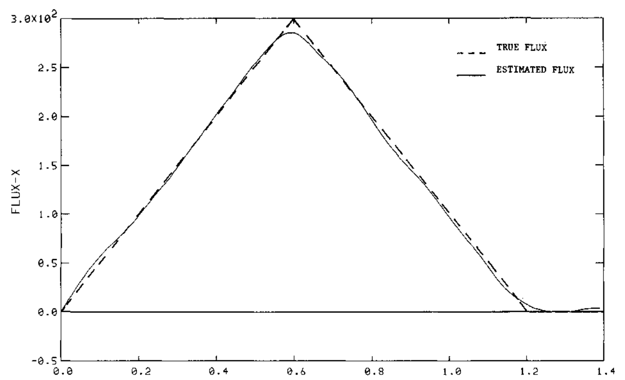


Fig. 10 Heat flux 1 for example 2, first-order regularization ($b = 1.137E - 6$).

the value of $b$ indicated by minimizing $V(b)$ ($b = 8.79E - 5$), one would obtain the heat fluxes shown in Figs. 7 and 8. Although the results are noisy, they still reflect the true nature of the unknown heat fluxes.

One technique for smoothing the unknown heat fluxes is first-order regularization (see Ref. 1). This is done by adjoining the following equations to the system of equations (1)

$$\dot{q}_1 = r_1 \qquad \dot{q}_2 = r_2 \tag{23}$$

The new system becomes

$$\begin{bmatrix} C & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} \dot{T} \\ \dot{q} \end{bmatrix} = \begin{bmatrix} K & P \\ 0 & 0 \end{bmatrix} \begin{bmatrix} T \\ q \end{bmatrix} + \begin{bmatrix} 0 \\ I \end{bmatrix} [r] \tag{24}$$

and the error expression [Eq. (7)] becomes

$$E_N(T_0, r_j) = \sum_{j=1}^{N} (z_j - d_j, z_j - d_j) + b(r_j, r_j) \tag{25}$$

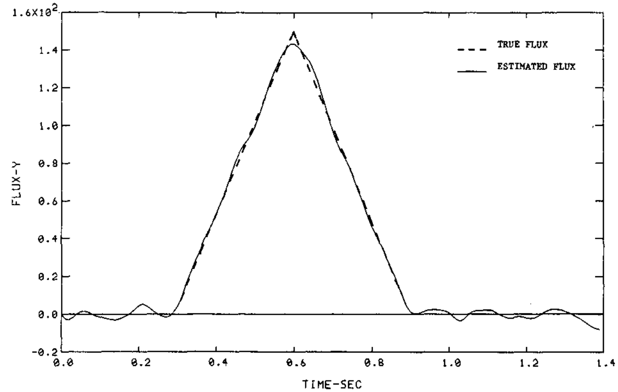


**Fig. 11 Heat flux 2 for example 2, first-order regularization ($b = 1.137E-6$).**

This increases the order of the system by only two. The regularization parameter is now applied to $r_1$ and $r_2$, which are now the unknown functions in the minimization problems.

The results using first-order regularization are shown in Fig. 9, which shows that $V(b)$ now successfully estimates the optimal regularization parameter $b^*$. The resulting heat fluxes are shown in Figs. 10 and 11. They are now very smooth and excellent representations of the true heat fluxes.

## Conclusions

The method of generalized cross validation (GCV) has been shown by numerical examples to give an excellent estimate of the optimal regularization parameter under certain conditions. Since GCV requires no information other than the data at hand and the model, it should be very useful in real situations.

One way to use this method is to perform simulations of a real situation using rough estimates of the heat flux. The simulation could vary the noise levels in the simulated data to obtain the effects on the functions $V(b)$ and $S(b)$. In addition, the first-order regularization could be used if necessary. Choosing the order of regularization beforehand is difficult. One guideline is that if the heat fluxes still appear "noisy" after selecting the parameter $b$ by minimizing $V(b)$, then a first-order (or higher) regularization may yield better results. This is due to the fact that the higher-order regularizations are on the derivatives of the heat fluxes and will always tend to smooth out the fluxes.

Although a few numerical examples are not enough to determine a method's validity, GCV shows much promise for estimating the optimal value of the regularization parameter. This is especially true since there are so few other methods available.

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