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OPTIMAL REGULARIZATION OF THE INVERSE-HEAT CONDUCTION PROBLEM USING THE L-CURVE

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ABSTRACT

Solving the inverse heat conduction using Tikhonov regularization requires the selection of an optimal smoothing parameter. One popular method for choosing the smoothing parameter is the generalized cross-validation method. This method works very well but is computationally expensive. In this paper we investigate the L-curve method for selecting an optimal smoothing parameter. This L-curve is easily computed and may prove very useful for large systems which preclude other methods.

KEY WORDS L-curve method Optimal regularization

INTRODUCTION

The inverse heat-conduction problem is concerned with the estimation of unknown heat fluxes based on measured transient temperature data. This is a very difficult problem and falls into a class of problems called ill-conditioned because the solution is extremely sensitive to the noise that is always present in the measurements. One very successful approach to these problems is to combine several rather abstract mathematical concepts, which, together, produce practical and excellent solutions to these problems. These are:

(1) least squares minimization with regularization (sometimes referred to as Tikhonov's method);
(2) dynamic programming, which provides a very efficient method for solving the regularized least squares problem;
(3) L-curve method or generalized cross-validation to select the optimal regularization parameter.

The use of generalized cross-validation (GCV) to select the regularization parameter has been previously investigated by Trujillo and Busby[1,2]. GCV worked extremely well, but requires the computation of the trace of a global solution matrix that relates all of the measurements to the estimated temperatures. When dealing with finite element models with thousands of nodes this method becomes computationally expensive and impractical. For this reason, the L-curve

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method, recently proposed by Hansen[3], may prove to be very useful. Hanson also indicates that for certain types of correlated noise the GCV method may fail while the L-curve will succeed. This paper investigates, numerically, the use of the L-curve to select the regularization parameter for a finite element inverse heat conduction problem. Two examples are included: a simple two-dimensional one with simulated data and an experimental one with real data. A complete description of the problem and methods is also included.

MATHEMATICAL MODEL

The mathematical model is very general and represents a dynamic system with the following vector–matrix difference equation:

$$\mathbf{x}_{j+1} = \mathbf{M}\mathbf{x}_j + \mathbf{P}\mathbf{q}_j \tag{1}$$

where $\mathbf{x}$ represents the temperature vector of length n. In our examples, $n = 25$ and 400, and in some practical problems n can easily reach 1000. $\mathbf{M}$ is a matrix which represents the dynamics of the model, $\mathbf{q}$ is a vector of length n_q representing the unknown heat fluxes, and $\mathbf{P}$ is matrix $(n \times n_q)$ relating the fluxes to the system. Typically, n_q is much less than n. A timestep h represents the difference between the temperature states $\mathbf{x}_j$ and $\mathbf{x}_{j+1}$. The timestep also equals the sampling increment of the data.

Measurements

Now suppose that a series of measurements have been taken and are represented by the vectors $\mathbf{d}_j$, where the length of $\mathbf{d}_j$ is m. The number of measurements m is usually much less than the number of variables n but greater than n_q. These measurements are related to the temperature $\mathbf{x}_j$ by:

$$\mathbf{d}_j \propto \mathbf{U}\mathbf{x}_j \tag{2}$$

where $\mathbf{U}$ is an $(m \times n)$ matrix which associates the measurements to the temperature vector.

Statement of the problem

The problem is to find the unknowns q_j that when used in (1) will force the model to best match the measurements represented by (2). It quickly becomes obvious that an exact match will not work. This is due to the fact that all measurements have some degree of noise while the models, on the other hand, have usually assumed all kinds of derivatives and smoothness. The most common method of adjoining the data to the model is with the use of least squares. In vector form this is represented with a vector inner product $(\cdot, \cdot)$ and would be represented by an error sum over all the data points N:

$$E = \sum_{j=1}^{N} (\mathbf{d}_j - \mathbf{U}\mathbf{x}_j, \mathbf{d}_j - \mathbf{U}\mathbf{x}_j)$$

Even this least squares criteria is not sufficient because a mathematical solution that will minimize E will usually end up with the model exactly matching the data. A situation that is to be avoided because the inverse problem is ill-conditioned, and the estimated heat fluxes are extremely sensitive to the data. This is where the regularization method enters. By adding a term to the above least squares error:

$$E = \sum_{j=1}^{N} \{(\mathbf{d}_j - \mathbf{U}\mathbf{x}_j, \mathbf{d}_j - \mathbf{U}\mathbf{x}_j) + b(\mathbf{q}_j, \mathbf{q}_j)\} \tag{3}$$

one can control the amount of smoothness that occurs in the solution by varying the parameter b. This method is sometimes referred to as Tikhonov's method. What is now required of the solution is to best match the data (the first term of (3)) but to have some degree of smoothness (the second term of (3)). This immediately brings up the question of what should be the value of the smoothing parameter b. In this paper we will investigate the use of the L-curve method.

L-CURVE METHOD

Hansen[3] presents the L-curve method in a general linear algebraic setting where one wishes to minimize the norm of the residual vector adjoined (via a parameter) with a semi-norm of the solution. This is known as Tikhonov regularization. The semi-norm usually represents a numerical approximation to the second derivative of the solution. The L-curve is a plot of the semi-norm of the solution *versus* the residual norm. Hansen points out that the practical use of this plot was first suggested by Lawson and Hanson[4]. With some assumptions, Hansen's analysis shows that L-curve will depend continuously on the smoothing parameter and that it will always have a corner and that a point slightly to the right of the corner estimates the optimal smoothing parameter. This corner is most easily seen in a log–log plot.

In our formulation of the inverse problem the residual norm corresponds to the first term of (3) which represents the error in matching the data. The semi-norm of the derivative of the solution corresponds to the second term of (3) or alternatively, the derivative of the heat fluxes. In a general formulation of the inverse problem, it is possible to replace the regularization term with a derivative of the heat fluxes in place of the heat fluxes themselves. This is easily accomplished by adjoining the heat fluxes to the state variables and solving for the derivatives of the heat fluxes (see Reference 1 for more details). Thus, in our application, the following norms will be plotted to produce the L-curves:

$$\mathbf{E}^2_{\text{norm}} = \frac{1}{N} \sum_{j=1}^{N} (\mathbf{d}_j - \mathbf{U}\mathbf{x}_j, \mathbf{d}_j - \mathbf{U}\mathbf{x}_j) \tag{4}$$

$$F^2_{\text{norm}} = \frac{1}{N} \sum_{j=1}^{N} (\mathbf{r}_j, \mathbf{r}_j) \tag{5}$$

where $\mathbf{q}_{j+1} = \mathbf{q}_j + \mathbf{r}_j$.

NUMERICAL EXAMPLE

This example was investigated in Reference 1 and represents a two-dimensional finite element model involving two unknown heat fluxes and two temperature measurements. *Figure 1* shows the model and the location of the measurements. A 0.4×0.8 rectangle was modelled with 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 0.01 units was used. A noise level of 0.5 degrees was added to the simulated measurements, which varied from 0 to 336 degrees.

The regularization problem was solved using several values of the smoothing parameter b. The results are shown in *Figure 2* which plots the F_{norm} *versus* the E_{norm} on log–log scales. The L shape characteristic of the curve is indeed present. The values of the smoothing parameter are shown for the data in the proximity of the corner. It only remains to validate that the optimal value of the smoothing curve does occur at the corner.

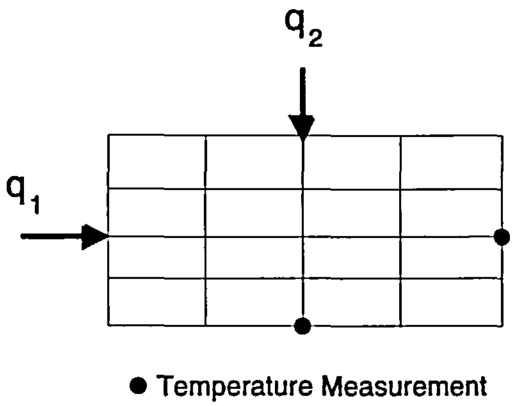

Figure 1 Finite element model and the location of the temperature measurements for example 1

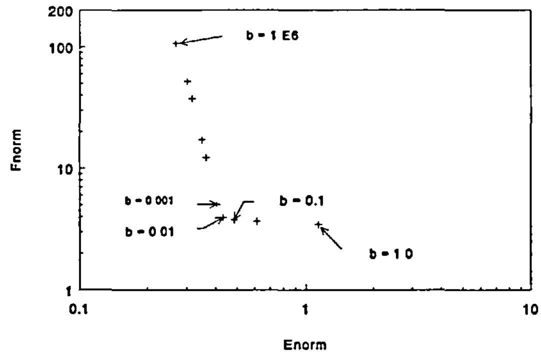

Figure 2 L-curve, F_{norm} *versus* E_{norm}. +, Data

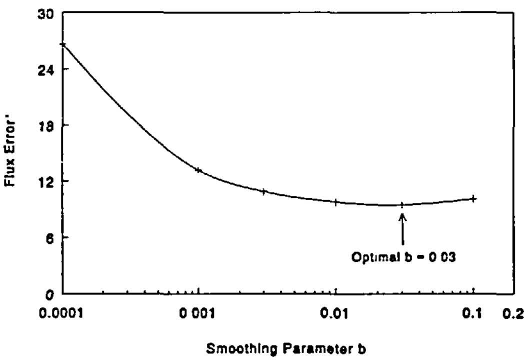

Figure 3 True flux error *versus b.* +, Data

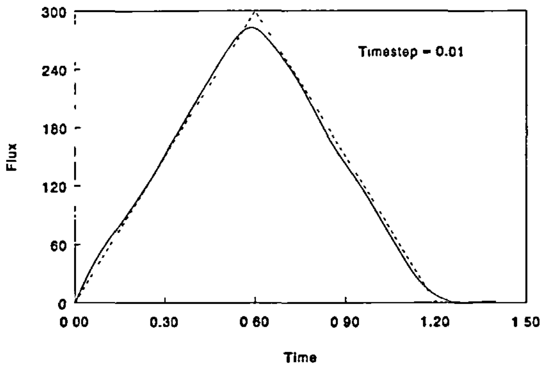

Figure 4 Estimated and true flux 1.——, b = 0.01; ----, true

One advantage of testing methods and theories with simulated data is that one knows the answer beforehand. *Figure 3* shows a plot of the least squares error between the *true* heat fluxes and the estimated ones for various smoothing parameters. From this Figure, the optimal smoothing parameter would be chosen as 0.03. From *Figure 2*, the corner of the L-curve is judged to be at 0.01. The estimated heat fluxes are not extremely sensitive to the parameter and either of these values would yield excellent estimates of the heat fluxes. The estimated and true heat fluxes are shown in *Figures 4* and *5* for the smoothing parameter of 0.01.

EXPERIMENTAL DATA

This example is taken from Trujillo and Wallis[5] and represents real data. A quenching experiment was carried out with an instrumented disk, (10.5 in. diameter × 2.75 in. thick) made from Alloy 718. The disk was heated to 2150°F in a gas-fired furnace before being transferred to an oil tank where it is quenched. An axisymmetric finite element model consisting of 400 nodes (n = 400) was used to represent the disk. Ten thermocouples (m = 10) were placed in the disk to capture the transient data. The finite element model and the locations of the thermocouples are shown

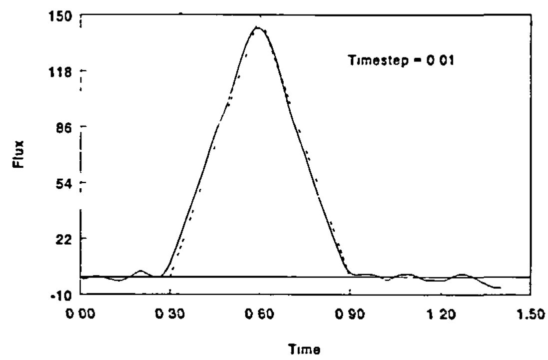

Figure 5 Estimated and true flux 2. ——, $b = 0.01$; ----, true

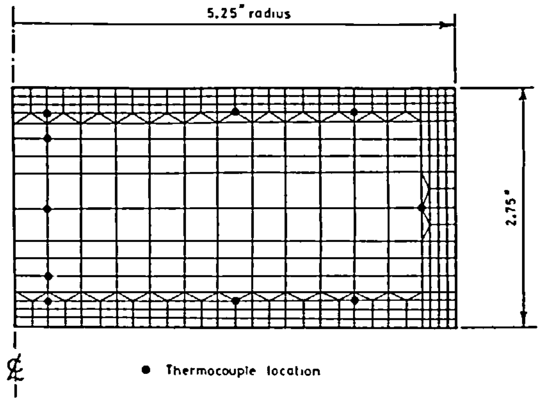

Figure 6 Axisymmetric finite element model showing the locations of temperature measurements

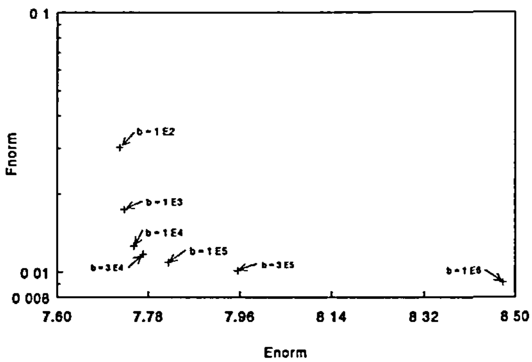

Figure 7 L-curve, experimental data. +, Data

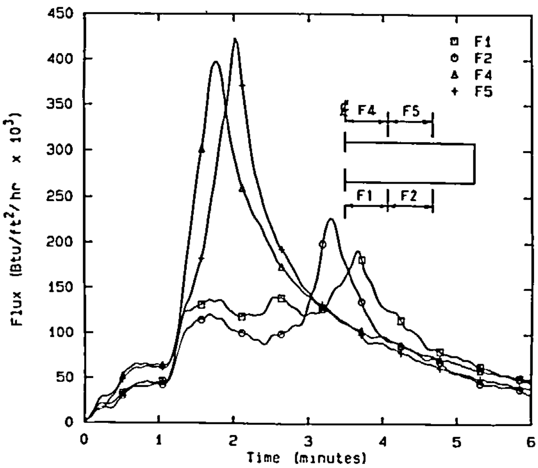

Figure 8 Variation of heat flux with time for the centre area of the disk

in *Figure 6*. The model was then used to estimate seven heat flux histories ($n_q = 7$) around the perimeter of the disk. The thermocouples were sampled every 2 sec for a total of 180 points ($N = 180$). Also, this problem is non-linear because of the temperature dependence of the thermodynamic properties of the metal.

The L-curve was constructed by solving the regularization problem using several values of the smoothing parameter b. The results are shown in *Figure 7* which plots the F_{norm} *versus* the E_{norm} on a log–linear scale. For this case the E_{norm} did not vary much in magnitude. However, the L shape characteristic of the curve is indeed present. Since this case represents real data there is no 'true' answer to help evaluate the performance of the L-curve, but the point slightly to the right of the corner value ($b = 1 \times 10^5$) corresponds very well to the value of the smoothing parameter that was chosen[5] based on experience and intuition. Four of the seven estimated heat fluxes are shown in *Figure 8*. These heat fluxes are for the center region of the disk, both top and bottom.

DISCUSSION

The results of the above examples gives one confidence that the L-curve is indeed a good method for selecting the optimal smoothing parameter. As Hansen indicates, the L-curve and generalized cross-validation would give the same parameter for most cases with white noise and even with filtered white noise. The main advantage of the L-curve method is that it can be plotted with readily available information, while constructing the GCV curve requires some additional computations. Thus, in computer programs that solve very large models the L-curve method is the only available practical method as was the case for the experimental model with 400 nodes and seven unknown heat fluxes.

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