Research Journal of Applied Sciences Engineering and Technology 4(9): 1131-1136, 2012
ISSN: 2040-7467

Submitted: December 02, 2011 Accepted: December 23, 2011 Published: May 01, 2012

Determination of an Unknown Radiation Term in a Nonlinear Inverse Problem using Simulation of Markov Chains

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Abstract: The purpose of the present study is to provide a fast and accurate algorithm for identifying the medium temperature and the unknown radiation term from an overspecified condition on the boundary in an inverse problem of linear heat equation with nonlinear boundary condition. The design of the paper is to employ Taylor's series expansion for linearize nonlinear term and then finite-difference approximation to discretize the problem domain. Owing to the application of the finite difference scheme, a large sparse system of linear algebraic equations is obtained. An approach of Monte Carlo method is employed to solve the linear system and estimate unknown radiation term. The Monte Carlo optimization is adopted to modify the estimated values. Results show that a good estimation on the radiation term can be obtained within a couple of minutes CPU time at pentium IV-2.4 GHz PC.

Key words: Finite difference scheme, Markov chain, Monte Carlo method, nonlinear inverse problem, radiation term

INTRODUCTION

The problem of determining unknown parameters in parabolic differential equations has bean treated by many authors (Cannon and Zachmann, 1982; Dehghan, 2002; Chen *et al*., 2001; Ebrahimi, 2011). Usually this problems involve the determination of a single unknown parameter from overspecified boundary data. In some applications, however, it is desirable to be able to determine more than one parameter from the given boundary data (Cannon, 1984; Chen *et al*., 2002; Ebrahimi *et al.*, 2008). It is well known that the radiative heat is a function of temperature. In certain radiative heat transfer it is of interest to devise methods for evaluating radiations function by using only measurements taken outside the medium. To date various methods have been developed for the analysis of the parabolic inverse problems involving the estimation of boundary condition or diffusion coefficient from measured temperature inside the material (Friedman, 1964; Cannon and Duchateau, 1980; Shidfar *et al*., 2006; Ivaz and Nikazad, 2005; Dehghan and Tatari, 2008; Farnoosh and Ebrahimi, 2010). For example in the work of Shidfar *et al*. (2006) a numerical algorithm based on finite difference method and least-squares scheme for solving a nonlinear inverse diffusion problem is applied. Also, Ivaz and Nikazad (2005) have studied the uniqueness of the solution of an inverse solidification of pure substance problem in two dimensions. It can be found that the numerical method proposed by Dehghan (2003), applied to a one-dimensional parabolic inverse problem. The results show that the accuracy of this study are very reasonable. Other numerical methods for solving semi-linear parabolic inverse problems have been proposed including the finite difference method presented by Dehghan (2002) and the He's variational iteration method investigated by Dehghan and Tatari (2008). The literature reviews showed that Wang and Zabaras (2004) successfully applied a Bayesian inference approach to the inverse heat coonduction problem. Recently Ebrahimi *et al*. (2008), employed Monte Carlo method in conjunction with finite difference scheme for solving a linear parabolic inverse problem in two-dimensional case. This paper seeks to determine an unknown radiation function which is depend on the heat in a radiative heat transfer equation. It is assumed that no prior information is available on the functional form of the unknown radiation term in the present study, thus, it is classified as the function estimation in inverse calculation. The unknown radiation term is approximated by the polynomial form and the present numerical algorithm is employed to find the solution. According to latest information from the research works it is believed that the solution of the present inverse problem with an unknown radiation term at boundary condition based on numerical-probabilistic algorithm included the Monte Carlo optimization has been investigated for the first time in the present study.

Description of the problem: We consider the problem of determining function $U(x,t)$ satisfying:

$$U_t = U_{xx},\ 0 < x < 1,\ 0 < t < T \quad (1)$$

$$U(x,0) = f(x), 0 \le x \le 1 \quad (2)$$

$$U(0,t) = g(t), 0 < t < T \quad (3)$$

$$U_x(1,t) - P(U(1,t)) = \chi(t),\ 0 < t < T \quad (4)$$

where T is a given positive constant.We consider problem (1)-(4) as a direct problem. The direct problem considered here is concerned with the determination of the medium temperatures when the radiation term P(U), the initial condition f(x) and the boundary conditions g(t) and $\chi(t)$ are known continuous functions on their domains. The direct problem (1)-(4) has a unique solution (Friedman, 1964).

For the inverse problem, the radiation term p(U), is regarded as being unknown. In addition, an overspecified condition is also considered available. To estimate the unknown coefficient P(U), the additional information of measurements on the boundary x = x_1, 0 < x_1< 1, is required. Let the temperature measurements taken at x_1=1 over the time period (0,T) be denoted by:

$$U(1,t) = \phi(t), 0 < t < t_f \quad (5)$$

It is evident that for an unknown function P(U), the problem (1)-(4) is under-determined and we are forced to impose additional information (5) to provide a unique solution pair (U, P(U)) to the inverse problem (1)-(5). We note that the measured temperature $U(1,t) = \phi(t)$ should contain measurement errors. Therefore the inverse problem can be stated as follows:

> By utilizing the above-mentioned measured temperature data, estimate the unknown function P(U) over the entire space and time domain. Certain types of physical problems can be modeled by (1)-(5). The Eq. (1) may be used to describe the flow of heat in a rod. Hence, we might think of this problem as the problem of determining the unknown radiation term in a rod.

METHODOLOGY

The application of the present numerical method to find the solution of problem (1)-(5) can be described as follows:

Linearizing the nonlinear term : For linearized nonlinear term in Eq. (4) we used Taylor's series expansion. Let $\Psi(\xi_1,\ldots,\xi_s)$ infinite differentiable nonlinear function of $\xi_1,\ldots,\xi_s$, then its Taylor's series expansion is given as

$$\psi(\xi_1,\ldots,\xi_s) = \psi(\bar{\xi}_1,\ldots\bar{\xi}_s) + \sum_{\delta=1}^{s} \frac{\partial \psi}{\partial \xi_\delta}(\bar{\xi}_1,\ldots\bar{\xi}_s)(\xi_\delta - \bar{\xi}_\delta) \quad (6)$$

where the overbar denotes the previously iterated solution. The function P(U) in Eq. (4) can be linearized by (6), as follows:

$$P(U) = P(\bar{U}) + \left(\frac{\partial}{\partial U} P(U)\right)_{U=\bar{U}}(U - \bar{U}) + 0((U - \bar{U})^2) \quad (7)$$

Finite difference scheme: We use fully implicit finite difference scheme for discretizing Eq. (1). Therefore, the Eq. (1) is approximated at the mesh point (p,q) by the difference equation:

$$F_{p,q}(u) = \frac{u_{p,q+1} - u_{p,q}}{v} - \frac{u_{p-1,q+1} - 2u_{p,q_{+1}} + u_{p_{+1},q_{+1}}}{\mu^2} = 0 \quad (8)$$

and as a result, from Eq. (1) to (4) we obtain:

$$-ru_{p-1,q+1} + (1+2r)u_{p,q+1} - ru_{p-1,q+1} = u_{p,q} \quad (9)$$

$$u_{p,0} = f(p\mu), q = 0 \quad (10)$$

$$u_{0,q} = g(qv), p = 0 \quad (11)$$

$$\left(\frac{u_{n+1,q} - u_{n-1,q}}{2\mu}\right) - P(\bar{u}_n) - \left(\frac{\partial P}{\partial u}\right)u = \bar{u}_n(u_{n,q} - \bar{u}_n) = \chi(qv), p = n \quad (12)$$

where $x = p\mu$, $t = qv$, $n\mu = 1$, p = 1(1)n, q = 0(1)M and $r = \frac{v}{h^2}$. Problem (9)-(12) may be written in the following matrix form:

$$A\Theta = B, \quad (13)$$

where,

$$A = \begin{bmatrix} 1+2r & -r & 0 & 0 & \\ -r & 1+2r & -r & 0 & \\ . & . & \ldots & . & \\ 0 & -r & 1+2r & -r & \\ 0 & 0 & -2r & 1+2r & -2r\mu\frac{\partial P}{\partial u}(\bar{u}_N) \end{bmatrix}$$

and

$$\Theta^t = \left(u_{1,q+1}\ \ u_{2,q+1}\ .\ .\ .\ u_{n-1,q+1}\ \ u_{n,q+1}\right).$$

Also,

$$B^t = \left(u_{1,q} + ru_{0,q+1}\ \ u_{2,q}\ .\ .\ .\ u_{n-1,q}\ \ u_{n,q} + \Omega\right)$$

in which

$$\Omega = 2r\mu P(\bar{u}_n) - 2r\mu\bar{u}_n\frac{\partial P}{\partial u}(\bar{u}_n) + 2r\mu\chi(qv + v)$$

Theorem 1: The finite difference scheme (8) is unconditionally stable, (Ebrahimi *et al*., 2008).

Theorem 2: The finite difference scheme (8) is consistent with the parabolic partial differential Eq. (1), (Ebrahimi *et al*., 2008).

From Theorems 1 and 2 and Lax s' equivalence theorem it obviously follows that u converges to *U* as μ tends to zero.

Solution of linear systems: To solve the linear system (13), we consider the following iterative method:

$$u_{i,q+1}^{(k)} = (1-\gamma)u_{i,q+1}^{(k-1)} + \frac{\gamma}{Aii} \{b_i - \sum_{j=1}^{i=1} A_{ij}u_{j,q+1}^{(k)} - \sum_{j=i+1}^{n} A_{ij}u_{j,q+1}^{(k-1)}\} \quad (14)$$

where $i = 1,\ldots,n$ and $\gamma \in (0,1]$. Which is called the Jacobi overrelaxation iterative method with relaxation parameter $\gamma \in (0,1]$. Equation (14) may be written in the following matrix form:

$$\Theta^{(k)} = L\Theta^{(k-1)} + f, k = 1,2,.... \quad (15)$$

where,

$$\Theta^{(k)} = \left(u_{1,q+1}^{(k)} \ldots\ldots u_{n,q+1}^{(k)}\right)^t$$

is the k-th iterative solution of (15), $L = I - DA$, $f = Db$ and!

$$D = diag\left(\frac{\gamma}{A_{11}},\ldots,\frac{\gamma}{A_{n,n}}\right),$$

is a diagonal matrix. In fact, we convert the system (13) into an equivalent system of the following form:

$$\Theta = L\Theta + f \quad (16)$$

Therefor, the sequence of approximate solution vectors of system (16) is generated by applying recursive Eq. (15). From (15) we obtain:

$$\Theta^{(k)} = f + Lf +,\ldots + L^{k-1}f + L^k\Theta^{(0)}, k + 1,2,....$$

If $\Theta^{(0)} = 0$, then:

$$\Theta^{(k)} = (I + L + \ldots + L^{k-1})f = \sum_{m=0}^{k-1} L^m f, k = 1,2,....$$

In the next section we compute the iterations $\Theta^{(k)} = 0$ using Monte Carlo method where k is a finite number.

Monte carlo method to solve linear system: The application of the present Monte Carlo method to find a solution of linear system (16) is as follows:

Consider the Markov chain

$$X = x_0 \to x_1 \to x_2 \to \ldots \to x_k \to \ldots \quad (17)$$

with state space {1, 2, … N} and transition matrix $P = p_{i,j}$, $i = j = 1,\ldots N$. Let $P(x_0 = i) = p_i$, $P(x_{N-1} = j \mid x_{N-2} = i) = P_{ij}$ where p_i and p_{ij} are the initial distribution and the transition probabilities of the Markov chain, respectively. The weight function W_m, for Markov chain (17) with N states, is defined by using the recursion formula:

$$W_0 = 1, W_m = W_{m-1}\frac{l_{x_{m-1,m}}}{P_{x_{m-1,m}}}, m = 1, 2,....$$

Now the following random variable is defined:

$$\Gamma_k[H] = \frac{H_{x_0}}{p_{x_0}} \sum_{m=0}^{k} W_m c_{x_m}$$

which is associated with the sample path:

$$x_0 \to x_1 \to x_2 \to \ldots \to x_k$$

where k is a given integer number and $H^t = (h_1,\ldots,h_N)$ is a given vector. We also consider the problem of finding the inner product:

$$\langle H, \Theta \rangle = h_1 u_{1,q+1} + \ldots + h_N u_{N,q+1}$$

where $\Theta^t = (u_{1,q+1},\ldots,u_{N,q+1})$ is the numerical solution of the problem (1)-(5).

Theorem 3: The mathematical expectation value of the random variableis $\Gamma_k[H]$ equal to the inner product<H, $\Theta^{(k)}$>,i.e.,

$$E(\Gamma_k[H]) = < H, \Theta^{(k)} >$$

For proof of the Theorem 3 we refer to (Rubinstein, 1981).

Table 1: Results for $u_{p,q}$ example 1, with P = 1,… ,5

q	Error (p = 1)	Error (p = 2)	Error (p = 3)	Error (p = 4)	Error (p = 5)
1	$2.12/10^5$	$120/10^5$	$4.19/10^5$	$1.92/10^5$	$4.14/10^5$
10	$5.40/10^5$	$7.02/10^5$	$3.28/10^5$	$2.19/10^5$	$5.62/10^5$
100	$4.11/10^5$	$4.43/10^5$	$4.41/10^6$	$0.02/10^5$	$3.41/10^5$
500	$2.05/10^5$	$7.03/10^6$	$7.25/10^5$	$7.06/10^5$	$7.37/10^5$
1000	$9.08/10^5$	$6.74/10^5$	$4.05/10^5$	$7.12/10^5$	$6.41/10^5$

Table 2: Results for $u_{p,q}$ example 1, with P = 1,… ,5

q	Error (p = 6)	Error (p = 7)	Error (p = 8)	Error (p = 9)	Error (p = 10)
1	$2.45/10^5$	$4.10/10^5$	$3.24/10^5$	$1.08/10^5$	$2.24/10^6$
10	$1.90/10^5$	$3.08/10^5$	$5.18/10^5$	$3.04/10^5$	$0.52/10^5$
100	$0.91/10^5$	$4.18/10^5$	$5.19/10^5$	$4.29/10^5$	$0.09/10^5$
500	$5.42/10^5$	$6.17/10^5$	$8.50/10^5$	$6.16/10^6$	$2.13/10^6$
1000	$7.16/10^5$	$7.23/10^5$	$0.90/10^5$	$4.25/10^5$	$3.11/10^6$

Table 3: Results for $u_{p,q}$ example 2, with P = 1,… ,5

q	Error (p = 1)	Error (p = 2)	Error (p = 3)	Error (p = 4)	Error (p = 5)
1	$1.27/10^5$	$5.29/10^5$	$4.19/10^5$	$2.12/10^5$	$1.27/10^6$
10	$3.25/10^5$	$2.97/10^5$	$3.28/10^5$	$1.07/10^5$	$5.62/10^5$
100	$4.11/10^5$	$1.85/10^5$	$4.17/10^5$	$4.82/10^5$	$9.11/10^6$
100	$4.25/10^5$	$5.23/10^5$	$8.10/10^5$	$5.96/10^5$	$1.94/10^5$
1000	$6.06/10^5$	$8.94/10^6$	$5.16/10^5$	$6.12/10^5$	$2.14/10^5$

Table 4: Results for $u_{p,q}$ example 2, with P = 1,… ,5

q	Error (p = 6)	Error (p = 7)	Error (p = 8)	Error (p = 9)	Error (p = 10)
1	$1.87/10^5$	*1.10*$/10^5$	$3.19/10^5$	$114/10^5$	$1.03/10^6$
10	$4.40/10^5$	$5.93/10^5$	$3.94/10^5$	$0.07/10^4$	$5.62/10^6$
100	$5.71/10^5$	$6.22/10^5$	$6.17/10^5$	$3.72/10^5$	$0.01/10^6$
100	$4.05/10^5$	$6.03/10^5$	$9.10/10^5$	$1.06/10^6$	1.2210^5
1000	$2.66/10^5$	$6.94/10^5$	$8.14/10^5$	$0.01/10^4$	$2.93/10^6$

To estimate:

$$< H, \Theta^{(k)} >= h_1 u_{1,q+1}^{(k)} + \ldots + h_n u_{n,q+1}^{(k)}$$

we simulate N random paths:

$$x_0^{(s)} \rightarrow x_1^{(s)} \rightarrow x_2 \rightarrow \ldots \rightarrow x_k^{(s)} s = 1(1) N$$

each with the length of k , and evaluate the sample mean:

$$\Omega_k[H] = \frac{1}{N} \sum_{s=1}^{N} \Gamma_k^{(s)}[H] \approx E(\Gamma_k[H]) = <H, \Theta^{(k)}>$$

In fact, from Theorem 3 we conclude that $\Gamma_k[H]$ is an unbiased estimator of the inner product < H, $\Theta^{(k)}$>. It is readily seen that by setting:

$$H^t = (\underbrace{0,\ldots,0,1,0,\ldots,0}_{j})$$

we obtain:

$$< H, \Theta^{(k)} >= u_{j,q+1}^{(k)}, j = 1,\ldots,n$$

Hence Γ_k[H] is an unbiased estimator of the $u_{j,q+1}^{(k)}$

Monte carlo optimization technique: In this work the polynomial form is proposed for the unknown function P(U) before performing the inverse calculation. Therefore P(U) approximated as:

$$p^{app}(U) = c_0 + c_1 U + \ldots + c_\iota U^\iota$$

where $\{c_0, c_1, \ldots, c_\iota\}$ are constants which remain to be determined simultaneously. The unknown coefficients $\{c_0, c_1, \ldots, c_\iota\}$ can be determined in such a way that the following functional is minimized:

$$J(c_0, c_1, \ldots, c_\iota) = \int_{t=0}^{T} \left| U^{cal}(x_1, t; c_0, c_1, \ldots, c_\iota) - \phi(t) \right|^2 dt$$

here, $U_{p,q}^{cal}$ are the calculated temperatures on the plan at the grid locations (x_p,y_q). These quantities are determined from the solution of the direct problem given previously by using an approximated P^{app} (U) for the exact P(U). The estimated values of c_j , j = 0,1,… ,ι are determined until the value of $J(c_0, c_1, \ldots, c_\iota)$ is minimum. The computational procedure for estimating unknown coefficients a_j and b_i are described as follows:

Consider the following deterministic optimization problem:

$$\min_{A \in D \subseteq R^{\iota+1}} J(C) = J(C^*) = J^* \quad (18)$$

where J(C) is real-valued bounded function defined on $R^{\iota+1}$ and C = (c_0,c_1,…c_ι). It is assumed that J achieves its maximum value at a unique point C^*. The function J(C) may have many local maximum in $R^{\iota+1}$ but only one global maximum.

Random search algorithm: For solving problem (18) we consider the following random search algorithm:

- Generate ι+1-dimensional random variables Z_1, Z_2,… from and ι+1-dimensional normal distribution with zero mean and covariance matrix C that is Z ~ N (0,C) where Z = (Z_1, Z_2,…)
- Select an initial point. $C_1 \in R^{\iota+1}$
- Compute J(C_1)
- Set i = 1
- If $C_i + Z_i \in D \subseteq R^{\iota+1}$, go to step 8
- Set $C_i = C_{i+1}$
- Go to step 10
- Compute $J(C_i+Z_i)$
- If $J(C_i+Z_i) \leq J(Ci+Zi) \leq J(Ci) - \varepsilon$ then (where $\varepsilon > 0$) set $C_{i+1}=A_i+Z_i$.
  else
  set $C_i = C_{i+1}$
- If the stopping criterion is met, stop; otherwise, set $i = i+1$
- Go to step 5

NUMERICAL RESULTS AND DISCUSSION

Example 1: In this example let us consider the following inverse problem:

$$U_t = U_{xx},\ 0 < x < 1,\ t > 0 \quad (19)$$
$$U(x,0) = \cos(x),\ 0 < x < 1 \quad (20)$$
$$U(0,t) = \exp(-t),\ 0 < t < T \quad (21)$$
$$U_x(1,t) - P(U(1,t)) = -1 - (\cos(1) + \sin(1))\exp(-t),\ 0 < t < T \quad (22)$$

with the over specified condition:

$$U(1,t) = \cos(1)\exp(-t),\ 0 < t < T \quad (23)$$

The exact solution of this problem is U(x,t) =cos (x)exp(-t) and P(U)=1+U.

To solve the problem (19)-(23) by the present numerical method, the unknown function P(U) defined as the following form $P(U) = c_0 + c_1U$ and the computational procedure for estimating unknown coefficients c_j are repeated until $J(c_0, c_1) \leq \varepsilon$ where $\varepsilon = 0.0001$.

The comparison of the surface temperature distributions between the exact results $U(x = p\mu, t = qv)$ and the present numerical results $u_{p,q}$ are shown in Tables 1 and 2. The present numerical algorithm is applied for $\mu = 1/10$ and $v = 1/100$. The initial guess of $\{c_0, c_1\}$ is$\{0.2,0.2\}$ and $\bar{u}_p$ is 0.5. The estimated values of c_0 and c_1 are $c_0 = 0.997850$ and $c_1 = 1$.

Example 2: In this example let us consider the following inverse problem:

$$U_t = U_{xx},\ 0 < x < 1, > 0 \quad (24)$$
$$U(x,0) = \sin(x),\ 0 < x < 1 \quad (25)$$
$$U(0,t) = 0,\ 0 < t < T \quad (26)$$
$$U_x(1,t) - P(U(1,t)) = [-1 + \exp(-t)\cos(1) - \exp(-2t)\sin^2(1) - 1.],\ 0 < t < T \quad (27)$$

with the overspecified condition:

$$U(1t) = \sin(1)\exp(-t),\ 0 < t < T. \quad (28)$$

The exact solution of this problem is U(x,t) = sin (x) exp (-t) and P(U) $1+U^2$.

To solve the problem (24)-(28) by the present numerical method, the unknown function P(U) defined as the following form $P(U) = c_0 + c_1U^2$ and the computational procedure for estimating unknown coefficients c_i are repeated until $J(c_0,c_1) \leq \varepsilon$, where $\varepsilon = 0.0001$.The comparison of the surface temperature distributions between the exact results $U(x = p\mu, t = qv)$ and the present numerical results $u_{p,q}$ are shown in Tables 3 and 4. The present numerical algorithm is applied for, $\mu = 2/100$ and $v = \frac{1}{10000}$. The initial guess of$\{c_0,c_1\}$is$\{0.3,0.3\}$ and $\bar{u}_p$ is 0.4 . The estimated values of c_0 and c_1 are $c_0 = 1.005197$ and $c_1 = 0.999410$.

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