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Bayesian Inference Approach to Estimate Robin Coefficient using Hybrid Monte Carlo Algorithm

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Abstract

In this paper, a non-linear heat conduction problem is considered to identify the Robin coefficient using inverse method. The coefficient of heat transfer represents the corrosion damage, which is time dependent, is estimated for the surrogated data. The forward mathematical model is discretized using finite difference method and implicit scheme is incorporated for temperature time history. A powerful Bayesian framework is applied to obtain the estimates of unknown parameters and the uncertainty associated with the estimated parameter is represented as standard deviation. The sampling space is explored using a Hamiltonian Monte Carlo algorithm. The maximum a posterior, mean and standard deviation are obtained based on 10000 samples. Results prove that Bayesian Inference approach does provide accurate parametric estimation to the inverse heat problem.

Keywords: Bayesian Inference, Hamiltonian Monte Carlo, Inverse Heat Conduction, Parametric Estimation, Robin Coefficient

1. Introduction

The applications of Inverse Heat Transfer phenomenon are found in various branches of engineering and science including in chemical engineering. Determination of boundary conditions, thermal properties, unknown heat source, heat transfer coefficients, and emissivity is important for efficient thermal systems. It is inevitable that the majority of the Inverse Heat Transfer problems (IHTP) are unstable, ill-posed, and unsolvable as opposed to the direct problems.

There are several numerical methods proposed by researchers to estimate the unknown thermo-physical properties. A detailed parameter and function estimation process has been discussed in Ozisik and Orlande³. Onyango et al.² used boundary element method for parametric estimation. Parthasarathy and Balaji⁵ applied Bayesian inference approach for multi-mode heat transfer problems. Masson et al.⁴ had estimated the two dimensional heat transfer coefficient by applying the iterative regularization method.

Based on the literature review, it has been identified that the Robin coefficient is very essential while designing any thermal systems and it is often referred as corrosion damage. But very few works has been attempted to examine the Robin coefficient based on stochastic method. The Bayesian inference is a powerful framework wherein the prior information about the unknown parameter can be incorporated in it. So, a parabolic heat conduction problem is solved for the known convection boundary conditions and the unknown Robin coefficient is estimated with reasonable accuracy.

2. Mathematical Model of the Problem

To determine the Robin coefficient (ρ), the proposed mathematical model of the heat transfer problem is given as:

$$\frac{\partial \theta}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t), \quad (x,t) \in Q := (0,1) \times (0,t_f] \quad (1)$$

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$$\theta(x, \mathbf{0}) = g(x), \qquad x \in [0, \mathbf{1}] \tag{2}$$

$$\frac{\partial \theta}{\partial x}(0,t) + \rho(t)\theta(0,t) = \mathbf{h_0}(t) \quad t \in [0,t_f]$$
 (3)

$$\frac{\partial \theta}{\partial x}(1,t) + \rho(t)\theta(1,t) = \mathbf{h_1}(t) \quad t \in [0,t_f]$$
 (4)

Where $t_f > 0$, the final time which is fixed randomly. The functions g,h_0,h_1 are given, and θ represents the temperature, which is a function of x and $t \cdot \rho(t) \geq 0$ is the coefficient of heat transfer representing the corrosion damage and it is also a function of time. In general, it is always addressed as a Robin coefficient during energy interaction, subsequently; it acts as an interface and adds to the overall thermal resistance of the system. The problem becomes direct and well posed when $\rho(t)$ is known. In majority of the practical applications, the characteristics of this coefficient are unknown and thus require additional information to determine the physical process in a complete sense.

The measurement data is considered as,

$$Y(t) = \theta(1, t), \qquad t \in [0, t_f]$$
 (5)

Let $F(\rho)$ be the vector of the determined temperatures at x = 1. Thus by solving the following equation, the following solution is obtained for the inverse problem. $F(\rho) = Y(6)$

The proposed problem, like the other inverse problems, is an ill-posed and unsolvable problem. Large deviations from the exact solution may also emerge owing to the contamination of the measurement data with random errors. So, to deal with the instability of the problem, in this paper, Bayesian inference approach is used.

2.1 Numerical Implementation of the Direct Problem

The forward-finite difference method (FDM) is used to solve Eq. (6) and χ is discretised into M points, uniformly spaced, as shown below.

$$x_i = x_{i-1} + h, x_0 = 0,$$
 $x_M = 1,$ $i = 1, 2, ..., M,$ $h = \frac{1}{M}$

Also, the discretization of time t is given by,

$$t_n = t_{n-1} + \tau, t_0 = 0,$$
 $t_N = t_f,$ $n = 1,2...N,$ $\tau = \frac{t_f}{N}$ $t_n = t_{n-1} + \tau, t_0 = 0,$ $t_N = t_f,$ $n = 1,2...N,$ $\tau = \frac{t_f}{N}$

Where N is any positive integer.

Denoting θ_i^n as the approximate value of (x_i, t_n) , the FDM used to discretize equations (1) – (4) is as follows:

$$\begin{split} \frac{\theta_i^{n+1} - \theta_i^n}{\tau} &= \frac{1}{2h^2} \Big(\theta_{i-1}^n - 2\theta_i^n + \theta_{i+1}^n + \theta_{i-1}^{n+1} - 2\theta_i^{n+1} + \theta_{i+1}^{n+1} \Big), \\ \theta_i^1 &= g(x_i), \\ \frac{\theta_i^n - \theta_i^n}{h} + \frac{\theta_i^{n+1} - \theta_i^{n+1}}{h} &= [\rho(t_n)\theta_i^n + \rho(t_{n+1})\theta_i^{n+1}] - [h_0(t_n) + h_0(t_{n+1})] + \frac{h}{\tau(\theta_i^{n+1} - \theta_i^n)} \\ \frac{\theta_i^n - \theta_{M-1}^n}{h} + \frac{\theta_i^{n+1} - \theta_{M-1}^{n+1}}{h} &= -[\rho(t_n)\theta_i^n + \rho(t_{n+1})\theta_i^{n+1}] + [h_1(t_n) + h_1(t_{n+1})] + \frac{h}{\tau(\theta_i^{n+1} - \theta_i^n)} \end{split}$$

The above set of equations can be represented as a matrix equation as follows,

$$A\theta^{n+1} = B\theta^n + C,$$

$$\theta^1 = G$$
,

Where the matrices,

$$\theta^{n} = [\theta_{1}^{n}, \theta_{2}^{n}, \dots \dots \theta_{M}^{n}]^{T},$$

$$C = \frac{\tau}{h} [h_{0}(t_{n}) + h_{0}(t_{n+1}), 0, \dots \dots 0, h_{0}(t_{n}) + h_{0}(t_{n+1})]^{T},$$

$$G = [g(x_{1}), g(x_{2}), g(x_{2}) \dots \dots g(x_{M})]^{T},$$

And the matrices A and B are $(M \times M)$ tri-diagonal matrices with

$$1 + r + \frac{\tau}{h}\rho(t_{n+1}) - r = 0 = 0$$

$$-\frac{r}{2} - 1 + r - \frac{r}{2} = 0$$

$$0 = 0 - \frac{r}{2} - 1 + r - \frac{r}{2}$$

$$0 = 0 - \frac{r}{2} - 1 + r - \frac{r}{2}$$

$$0 = 0 - r - 1 + r + \frac{\tau}{h}\rho(t_{n+1})$$

$$1 - r - \frac{\tau}{h}\rho(t_{n+1}) - r = 0 = 0$$

$$\frac{r}{2} - 1 - r - \frac{r}{2} = 0$$

$$0 = 0 - \frac{r}{2} - 1 - r - \frac{r}{2}$$

$$0 = 0 - \frac{r}{2} - 1 - r - \frac{r}{2}$$

Where $=\frac{\iota}{h^2}$. Experimental temperature. For example,

$$Y = F(\rho) + \omega(7)$$

Where ω indicates the presence of random error, which can arise due to the errors in measurement. Now the solution to the inverse heat transfer problem is obtained by estimating the actual Robin coefficient $\rho(t)$ such that the determined temperatures $F(\rho)$ with this estimate can match the measurement temperatures Y.

3. Bayesian Inference Approach

Bayesian inference method is quite different from the deterministic methods in the way that they utilize all the prior information to obtain the posterior density function p(x/Y), where x is the quantity to be determined from the measurements Y. To quantify the quality of the result, any statistics about x can be determined. By the recent advancement of MCMC methods like Metropolis Hastings and Hybrid Monte Carlo, the Bayesian inference method has become very much beneficial due to its lesser computational time equivalent to deterministic methods.

Bayesian inference approach uses the Bayes law,

$$\pi(\rho|Y) = \pi(Y|\rho)\pi(\rho), \tag{8}$$

Where $\pi(Y|\rho)$, is the likelihood function and $\pi(\rho)$ is the prior. Hereby $\pi(.)$ indicates the probability density function (pdf). Through the prior distribution function $\pi(\rho)$ expert knowledge about the expected solution can be incorporated prior to any measurements. The likelihood function $\pi(Y|\rho)$ will have the knowledge about both the model and the noise.

In the Bayesian method, the construction of the likelihood function $\pi(Y|\rho)$ is the most direct part. Assuming a simple model, the random errors in (7) can be considered as they are independent and identically distributed.

Then the likelihood function is given by,

$$\pi(Y|\rho)\alpha\left(\llbracket\sigma^2\right)\rrbracket^{\frac{-y}{2}}\exp\left(-\frac{(F(\rho)-Y)^T(F(\rho)-Y)}{2\sigma^2}\right) \quad (9)$$

Where v is the dimension of the matrix v.

The main step is the construction of the prior density function which is used for prior modeling in Markov random field (MRF). For this work, following MRF is taken

$$\pi(\rho)\alpha\lambda^{\frac{m}{2}}\exp\left(-\frac{1}{2}\lambda\rho^TW\rho\right)$$
 (10)

With (9) and (10) the PPDF can be evaluated as follows,

$$\pi(\rho|Y)\alpha \exp\left(-\frac{(F(\rho) - Y)^T(F(\rho) - Y)}{2\sigma^2}\right) \exp\left(-\frac{1}{2}\lambda\rho^T W\rho\right)$$
(11)

Here, it is assumed that λ is the regularization parameter. m, is the dimension of the vector.

4. Hamiltonian Monte Carlo HMC

Hamiltonian Monte Carlo method reduces the correlation between successive sampled states by using Hamiltonian Dynamics between the states, which results in higher acceptance ratio and fast convergence to the solution.

The Hamiltonian is defined as sum of Potential Energy (U) and kinetic Energy (K).

$$H(x,p) = U(x) + K(p), \tag{12}$$

where 'x' is the location variable and 'p' is the momentum variable. For each position of 'x' there is a corresponding value of 'p'. Hamiltonian dynamics allows us to convert Kinetic energy into Potential Energy (and vice versa) as an object moves in time (t) using the following set of differential equations.

$$\frac{\partial x_i}{\partial t} = \frac{\partial H}{\partial p_i} = \frac{\partial K(p)}{\partial p_i} \tag{13}$$

$$\frac{\partial p_i}{\partial t} = -\frac{\partial H}{\partial x_i} = -\frac{\partial U(x)}{\partial x_i} \tag{14}$$

Therefore by knowing the initial values of 'x' and 'p' at a time 't_o', it is possible to predict value of 'x' and 'p' and another time 't = t_0 + T' by using Leap frog algorithm.

5. Leap Frog Algorithm

The step 2 in the procedure given below involves application of the leap frog algorithm. In practice, we cannot simulate Hamiltonian dynamics exactly because of the problem of time discretization. Leap frog is one of the many ways of trying to overcome this and thus simulate. It has the following steps:

1.
$$p\left(t + \frac{\Delta}{2}\right) = p_i(t) - \left(\frac{\Delta}{2}\right) \frac{\partial U(x)}{\partial x_i}$$
 (15)

2.
$$x_i(t + \Delta) = x_i(t) + (\Delta) \frac{\partial K(p)}{\partial p_i(t + \Delta)}$$
 (16)

3.
$$p_i(t + \Delta) = p_i \left(t + \frac{\Delta}{2}\right) - \frac{\left(\frac{\Delta}{2}\right) \partial K(p)}{\partial p_i(t + \Delta)}$$
 (17)

In parametric estimation, we replace the variable 'x' with the required parameter ρ . The following steps are taken to determine the estimation of the parameter.

- Initial guess of the robin coefficient o is taken.
- A momentum variable 'p' is taken for initiating the Leap frog Algorithm, which helps in sampling the given parameter ρ to the next state.
- · We denote 'u' as a variable of random value between 0 and 1.

- Let alpha be a minimum value of either 1 or
 e^{(U0+K0)-(Uf+Kf)}), where U0 and K0 are the
 potential and Kinetic energies at initial sample
 states; Uf and Kf are those of next sample state
 obtained in step 2, using Leap frog Algorithm.
- Using the condition for acceptance as follows:
 a. If u < alpha, then ρ f value is accepted.

b. If u >= alpha, then the new sample state value obtained in step 2 is not accepted and ρ remains the same as previous value.

• This entire procedure is iterated over number of samples required.

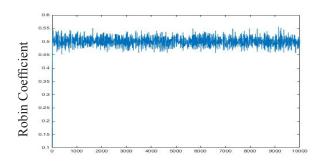
As the HMC converges, the recorded samples form the target posterior distribution function.

6. Experimental Results

In this section the efficiency and the accuracy of the Bayesian inference approach are explained by a numerical example. The following functions and values have been considered in the numerical experiment.

$$t_f = 1$$
 $g(x) = x^2 + 1$ $h_0(t) = t(2t + 1)$
 $h_1(t) = 2 + 2t(2t + 1)$

The problem is solved using MATLAB software. The length of the chain or the number of samples is taken to be 10000. The value of \hbar and τ are considered to be 0.1, by taking M and N as 10. λ , The regularization parameter is taken as 10.



Number of Samples

Figure 1. HMC Method of Sampling Robin coefficient at temperatures corresponding to its value of 0.5.

In this example the Robin coefficient is defined as a smooth function $\rho(t) = t$. Figure 1 shows the markov chain process. The initial guess

of the Robin coefficient is 0.1 and eventually it reached the solution within 100 samples. The advantage of the Bayesian framework along with HMC algorithm is, irrespective of the initial guess the process converges to the solution. Totally 10000 samples have been considered to obtain better mean and MAP estimates. The posterior probability density function is plotted against the 10000 samples and it is shown in Figure 2.

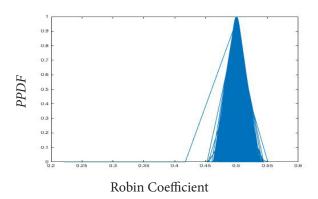
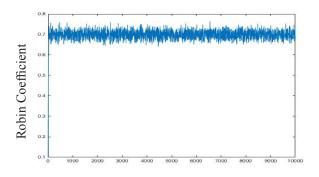


Figure 2. PPDF distribution of Robin coefficient at temperatures corresponding to its value of 0.5.

Similarly for temperatures corresponding to P = 0.7, we obtain the following convergence to 0.7 value.



Number of Samples

Figure 3. HMC Method of Sampling Robin coefficient at temperatures corresponding to its value of 0.7.

7. Future Work

In this paper the authors reinforced the work done by other researchers in the field of Bayesian inference there by determining the Robin coefficient of an inverse heat conduction problem. Hybrid Monte Carlo, is a proven algorithm in many fields of science that it is better than Metropolis Hastings in convergence of the solution and in the acceptance ratio. The future scope of the present work is to employ HMC in a similar fashion for the other inverse heat conduction problem and compare its performance with that of Metropolis Hastings.

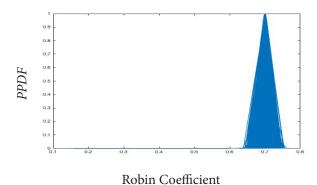


Figure 4. PPDF distribution of Robin coefficient at temperatures corresponding to its value of 0.7.

8. Conclusion

Bayesian inference approach is employed, in this paper, using the Hamiltonian Monte Carlo algorithm to identify a Robin coefficient in parabolic problems. 1-D transient conduction equation has been considered and convection boundary conditions were applied. Implicit scheme was incorporated to obtain the temperature distribution for the conduction problem. The Robin coefficient was estimated efficiently using HMC algorithm. The efficiency of

the Bayesian framework successfully tested for different initial guess and satisfactory results have been obtained. The results prove that the Bayesian inference approach can be used to obtain a near accurate solution to the parametric estimation problems.

9. References

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