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An Inverse Method for Simultaneous Estimation of Thermal Properties of Orthotropic Materials using Gaussian Process Regression

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Abstract. In this work, inverse heat conduction problem (IHCP) involving the simultaneous estimation of principal thermal conductivities (k_{xx}, k_{yy}, k_{zz}) and specific heat capacity of orthotropic materials is solved by using surrogate forward model. Uniformly distributed random samples for each unknown parameter is generated from the prior knowledge about these parameters and Finite Volume Method (FVM) is employed to solve the forward problem for temperature distribution with space and time. A supervised machine learning technique-Gaussian Process Regression (GPR) is used to construct the surrogate forward model with the available temperature solution and randomly generated unknown parameter data. The statistical and machine learning toolbox available in MATLAB R2015b is used for this purpose. The robustness of the surrogate model constructed using GPR is examined by carrying out the parameter estimation for 100 new randomly generated test samples at a measurement error of ± 0.3K. The temperature measurement is obtained by adding random noise with the mean at zero and known standard deviation ($\sigma = 0.1$) to the FVM solution of the forward problem. The test results show that Mean Percentage Deviation (MPD) of all test samples for all parameters is < 10 %.

1. Introduction

Parameter estimation using inverse method is widely practised in almost all engineering disciplines where direct measurement of the parameters is not feasible. For example in inverse heat conduction problems (IHCP) temperature measurements are used to estimate/identify boundary heat fluxes, thermo-physical properties, location and strength of heat sources[1]. However, inverse problems are ill-posed in nature. That is, a small measurement error in the *effect* (temperature in the case of IHCP) leads to the different/erroneous *cause* and sometimes the inverse problem may not be solvable at all. Therefore, the successful solution of any inverse problem relies on the optimal design of experimental parameters that enables high-quality measurement of *effect*, accurate modelling and solution of the forward problem that closely mimics the experimental configuration, suitable method for the solution of inverse problem that is robust enough for tackling ill-posedness arising due to measurement errors and multiple parameters.

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In literature, non-linear least square algorithms (with regularization scheme) such as Levenberg-Marquardt[2], Conjugate gradient[3] are used to solve the inverse problem. The major setback with these methods is that when multiple parameters are estimated simultaneously/ when the parameters are correlated, the solution converges to another feasible solution (local optimum). To overcome this, stochastic search techniques such as Genetic Algorithm[4] may be used to solve the inverse problem. Recently, methods based on statistical inversion such as Bayesian inference is used extensively due to its ability to incorporate prior beliefs about the parameter and measurement uncertainty in the inverse solution. However in this method, a large number of samples are required to approximate the posterior distribution with the sampling distribution and hence the forward problem has to be repeatedly solved for a large number of times. Sampling algorithms such as Markov Chain Monte-Carlo(MCMC), Gibbs sampler may be used to sample through the posterior distribution since the analytic way of calculating the expectations is difficult for multi-parameter space. In some cases (e.g., multi-parameter estimation), where a single solution of the forward problem alone requires huge computational time, an inverse solution using Bayesian/deterministic search methods takes months together. Also, in multi-parameter estimation at high measurement uncertainties efficient hybrid sampling techniques are required to sample through a posterior distribution[5], which again increases the computational time required for the solution of the inverse problem. In order to address these issues, surrogate forward models are used for the solution of the inverse problem. In the literature, the surrogate models are categorized into three different classes: data-fit models, reduced-order models and hierarchical models. A brief discussion about these models are presented in [6].

In this work, a methodology for solving inverse problem using surrogate model (data-fit model) is demonstrated. An inverse heat conduction problem is considered for demonstration in which five parameters say, principal thermal conductivity components of orthotropic materials, its specific heat capacity and heat transfer coefficient are identified simultaneously. The robustness of inverse parameter estimation with surrogate forward model constructed using GPR is examined by retrieving the parameters from the forward problem with noisy temperature measurement for 100 new test samples.

2. Definition of forward problem

The governing equation for heat conduction in a cuboid orthotropic material with constant heat flux boundary condition at one face and convection boundary condition on the remaining faces is regarded as the forward problem. Mathematically the forward problem is given by,

$$k_{xx}\frac{\partial^2 T}{\partial x^2} + k_{yy}\frac{\partial^2 T}{\partial y^2} + k_{zz}\frac{\partial^2 T}{\partial z^2} = \rho C_p \frac{\partial T}{\partial t} \quad in \quad -\frac{a}{2} \leq x \leq \frac{a}{2}, -\frac{b}{2} \leq y \leq \frac{b}{2}, 0 \leq z \leq c \tag{1}$$

subjected to the following initial and boundary conditions.

$$T(t=0,x,y,z) = T_i \quad in \quad -\frac{a}{2} \leq x \leq \frac{a}{2}, -\frac{b}{2} \leq y \leq \frac{b}{2}, 0 \leq z \leq c \tag{2}$$

$$q = \begin{cases} \mathrm{q}_0, & 0 \leq \mathrm{t} \leq t_0 \qquad \text{in the region} \quad \Gamma_1 \\ 0, & \mathrm{t} > \mathrm{t}_0 \end{cases} \tag{3}$$

$$n.(k_{ii}\nabla T_i) = h(T - T_\infty) \quad in\, the\, region \quad \Gamma_2, \Gamma_3, \Gamma_4, \Gamma_5\, and\, \Gamma_6 \tag{4}$$

where,

$$\Gamma_1 : -\frac{a}{4} \leq x \leq \frac{a}{4}, -\frac{b}{4} \leq y \leq \frac{b}{4}, z = 0 \quad \Gamma_2 : -\frac{a}{2} \leq x \leq \frac{a}{2}, -\frac{b}{2} \leq y \leq \frac{b}{2}, z = c$$
$$\Gamma_3 : x = -\frac{a}{2}, -\frac{b}{2} \leq y \leq \frac{b}{2}, 0 \leq z \leq c \quad \Gamma_4 : x = \frac{a}{2}, -\frac{b}{2} \leq y \leq \frac{b}{2}, 0 \leq z \leq c$$
$$\Gamma_5 : -\frac{a}{2} \leq x \leq \frac{a}{2}, y = -\frac{b}{2}, 0 \leq z \leq c \quad \Gamma_6 : -\frac{a}{2} \leq x \leq \frac{a}{2}, y = \frac{b}{2}, 0 \leq z \leq c$$

and a, b and c are the corresponding lengths (m) of the cuboid in x, y and z directions respectively. Similarly k_{xx}, k_{yy} and k_{zz} are constant thermal conductivity (W/mK) (independent of temperature) components along x, y and z directions respectively. Also ρ and C_p are density (kg/m^3) and specific heat capacity (J/kgK) respectively.

The boundary condition depicts that one face ($z = 0$ plane) is subjected to a localized heat flux of magnitude q_0 until time t_0 on the area enclosed by $-\frac{a}{4} \leq x \leq \frac{a}{4}, -\frac{b}{4} \leq y \leq \frac{b}{4}$ in Γ_1 and the heat that is being conducted within the solid domain under consideration is convected to the surrounding medium with heat transfer coefficient h (W/m^{2}K) and temperature T_∞ through the areas enclosed by the regions Γ_2 to Γ_6.

3. Gaussian Process Regression

Gaussian Process Regression (GPR) can be simply thought of as an ordinary Bayesian regression with an infinite dimensional parameter space of unknown nonlinear regression functions. Thus, the unknown nonlinear regression function is regarded as the unknown parameter, i.e., the random functions to be estimated and its prior distribution also needs to be specified. A specific probability distribution is considered for random functions and in general a multivariate standard normal distribution is most widely used[8].

Let $\mathbf{Z} \in \mathbb{R}^{n \times r}$ denotes a matrix, whose each column vectors are randomly generated samples for each unknown parameter. Here r=5, since there are five unknown parameters and let $\mathbf{X} \in \mathbb{R}^{n \times m}$ denotes a matrix whose elements are simulated temperature (solution of forward problem) with $\mathbf{Z}$ as input. i.e, $T(t, x, y, z)$. Let $\mathcal{D} = (\mathbf{X}, \mathbf{Z})$ denotes a data matrix available for GPR training.

The likelihood of $\mathcal{D}$ for a standard, one-dimensional, zero-mean GPR is given by[7],

$$p(\mathcal{D}|\theta) = \mathcal{N}_n(\mathbf{Z}|\mathbf{0_n}, \mathbf{A_n} + \sigma_\mathbf{s}^\mathbf{2}\mathbf{I_n}) \tag{5}$$

where $\mathbf{0_n} \in \mathbb{R}^{n \times 1}$ is the zero mean vector, $\theta = (\sigma_f^2, \sigma_l^2, \sigma_s^2)$ is the vector of all hyper-parameters. σ_f^2 and $\sigma_l^2 > 0$ are the parameters of covariance function, σ_s^2 is the noise level (in this work, it is assumed that σ_s^2=0) and $\mathbf{A}_\mathrm{n} \in \mathbb{R}^{n \times n}$ is the covariance matrix. In this work, Squared Exponential (SE) covariance function is used and it is given by:

$$\mathcal{K}(x_i, x_j|\sigma_f^2, \sigma_l^2) = \sigma_f^2 \exp\left(-\frac{1}{2}\frac{(x_i - x_j)^T(x_i - x_j)}{\sigma_l^2}\right) \tag{6}$$

where σ_f^2 and σ_l^2 are signal standard deviation and length scales respectively. Refer[8] for GPR training and prediction method for newly observed input data, $\mathbf{X}^* \in \mathbb{R}^{1 \times m}$

4. Results and Discussion

In this section, the results of parameter estimation using surrogate forward model is presented. As mentioned earlier, GPR training is used to construct the surrogate model. The range of unknown thermal properties in their respective units chosen for training are as follows:

$$0.1 \leq k_{xx} \leq 10, \quad 0.1 \leq k_{yy} \leq 2, \quad 0.1 \leq k_{zz} \leq 2,$$
$$1200 \leq C_p \leq 1800, \quad 5 \leq h \leq 18$$

The interval for all these parameters are usually chosen from the prior knowledge about the parameters. An arbitrary size of uniformly distributed random sample is generated for each unknown parameter and the forward problem is solved for temperature distribution $T(t, x, y, z)$ using Finite Volume Method (FVM) with these samples as input. The set of algebraic equations obtained by applying energy balance to each control volume is solved using Gauss-Seidel iterative technique. The heating time (t_0) and final time of experiment (t) is decided after studying the determinant of Fisher information matrix[2] for a fictitious but realistic orthotropic material[3] and from the results of such numerical test, the heating and final time of experiment is chosen to be 1080 and 1620 seconds respectively. In this work, all temperature solutions are considered only at z=c plane, which enables the use of non-intrusive method of temperature measurements in real time application. Now, with the simulated data $\mathcal{D} = (\mathbf{Z}, \mathbf{X})$ a surrogate forward

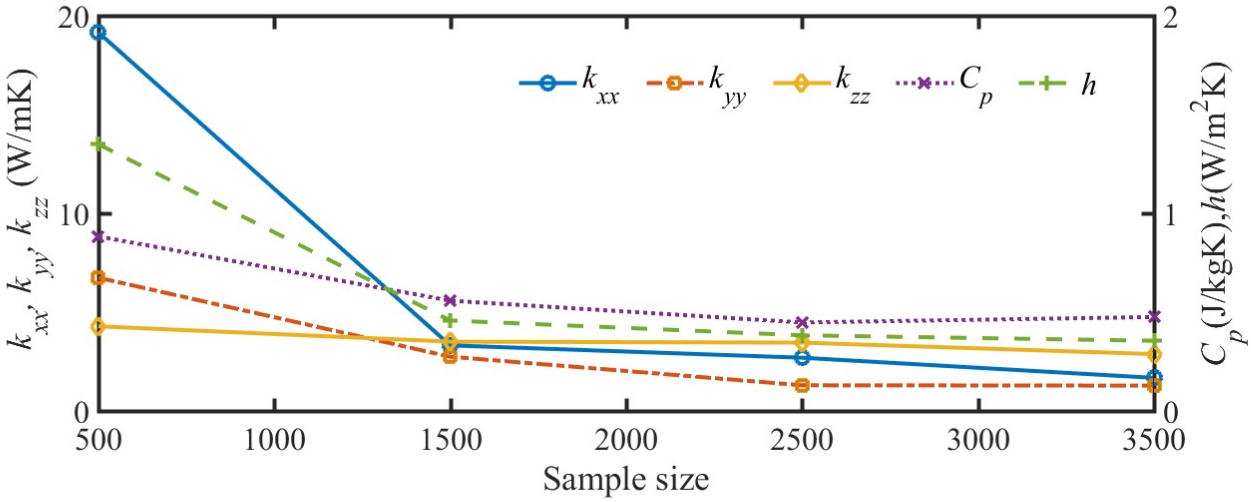

Figure 1. Sample vs MPD at measurement error=±0.03K.

model is constructed using GPR[8]. MATLAB R2015b is used for training and predicting the response for new input data $\mathbf{X}^*$. As mentioned earlier, Squared Exponential (SE) covariance function is chosen to represent the similarity kernel matrix for input data. The trained surrogate forward model is then used to estimate the unknown parameters with the simulated experimental temperatures as input. A total of 100 new samples for each parameter is considered for testing the trained surrogate model. The Mean of Percentage Deviation from actual value (MPD) for each unknown parameter is calculated using the equation (7).

$$\text{MPD} = \frac{1}{100} \sum_{i=1}^{100} \left\{ \frac{|y^i_{est} - y^i|}{y^i} \times 100 \right\} \tag{7}$$

In equation (7), y_{est} and y denotes the estimated parameter using trained surrogate model and actual parameter respectively. Figures 1 and 2 show the variation of MPD with sample size at measurement error of ±0.03K and ±0.3K respectively. As expected, the MPD for all parameters decreases with the increase in sample size. Therefore, a sample size of 3500 is considered in the further analysis, since the cumulative MPD of all parameters is less in this case and also with

[2] $\mathbf{F}$=$\mathbf{J}^T\mathbf{J}$, where $\mathbf{J}$ is the sensitivity matrix for the unknown parameters. Refer[1] for the definition of sensitivity matrix

[3] k_{xx}=5W/mK, k_{yy}=0.7W/mK, k_{zz}=0.6W/mK, C_p=1500J/kgK, h=10W/m^{2}K

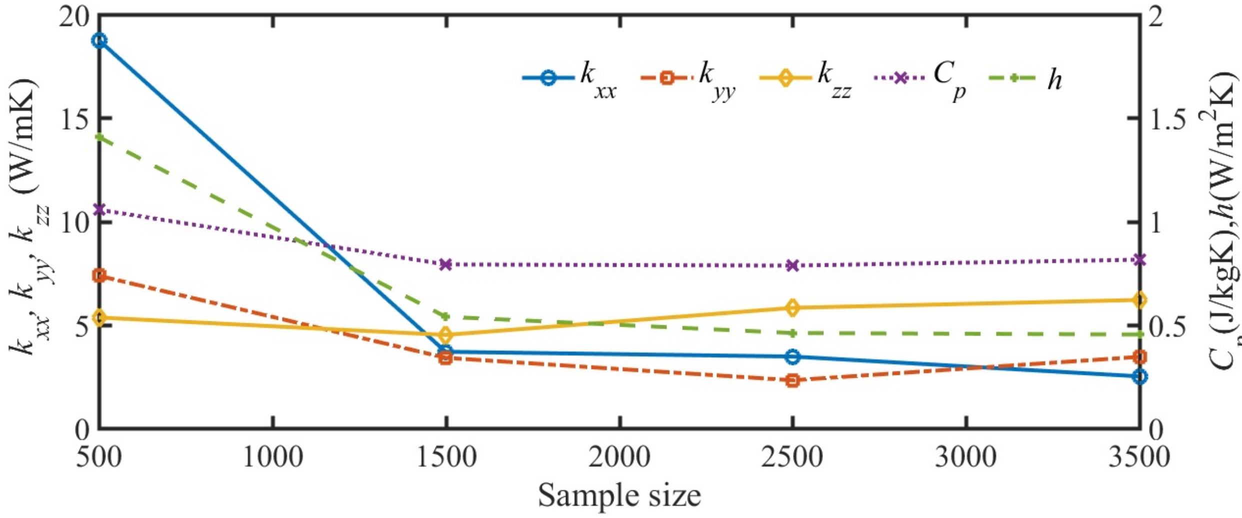

Figure 2. Sample vs MPD at measurement error=±0.3K.

further increase in sample size there is no significant change in MPD. From figures 1 and 2, it is clear that the MPD for all parameters is less at measurement error ±0.03K than at ±0.3K irrespective of the sample size. However, measuring temperature at this level of uncertainty is extremely difficult in real time experiments and hence only the results of estimation at ±0.3K is presented in the following sections.

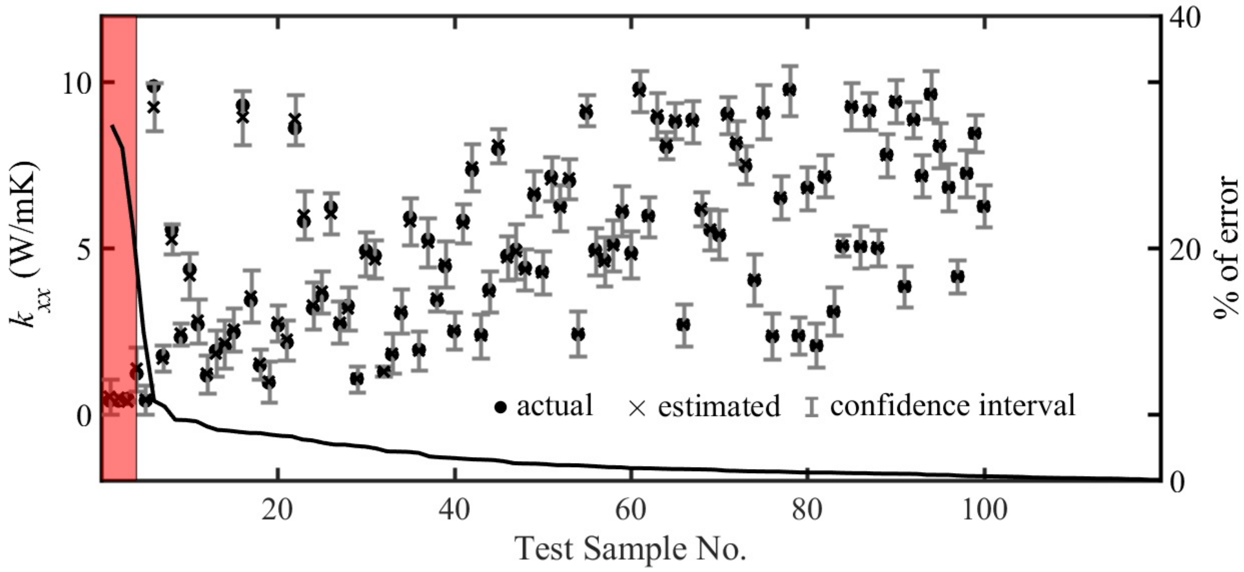

Figure 3. Estimated k_{xx} (W/mK) for 100 test samples. (shaded region includes the estimated samples with % of deviation > 10)

The results of parameter estimation for 100 new test samples using surrogate model for each unknown parameter at measurement uncertainty of ±0.3K is shown in figures 3 to 7 respectively. The percentage of deviation from the actual value for all 100 test samples is less than 10% in case of C_p and h which is clearly visible in figures 6 and 7. The number

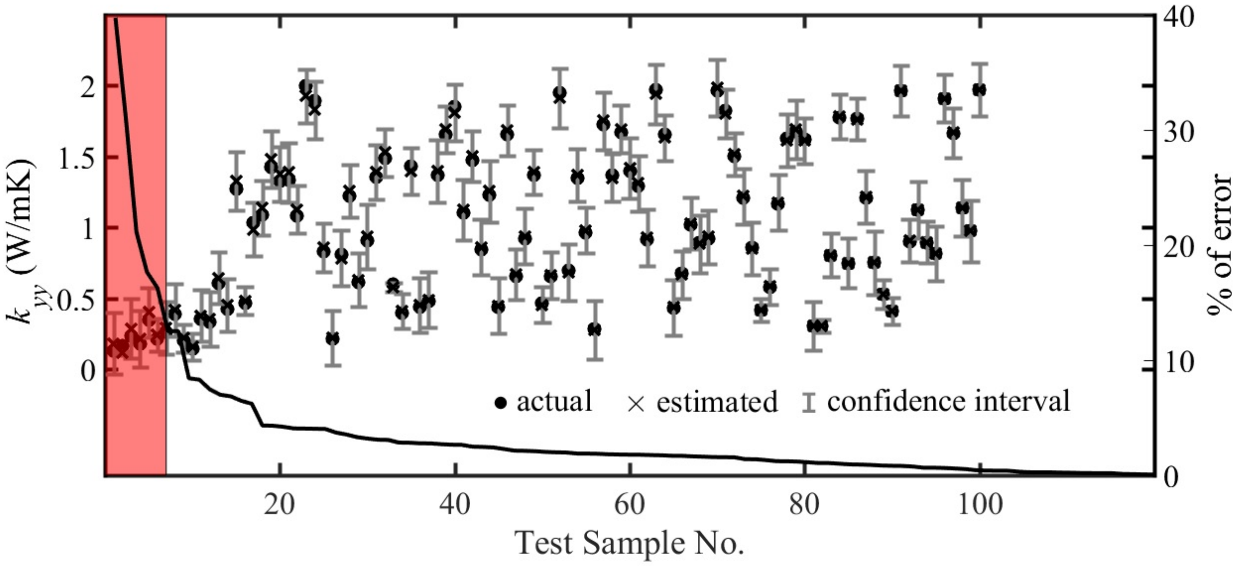

Figure 4. Estimated k_{yy} (W/mK) for 100 test samples. (shaded region includes the estimated samples with % of deviation > 10)

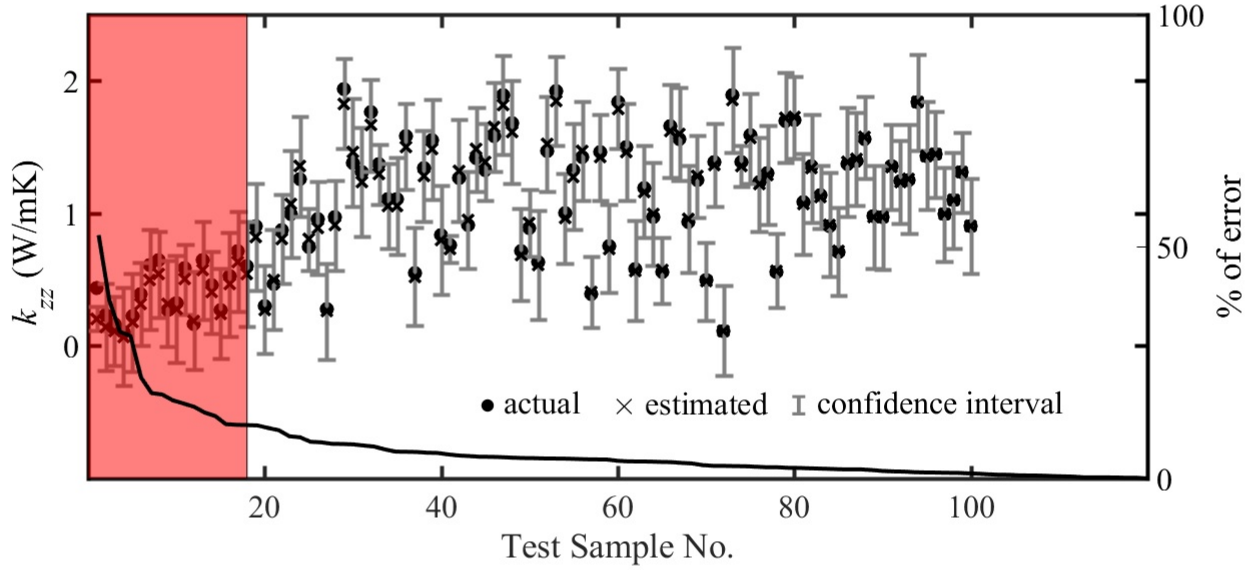

Figure 5. Estimated k_{zz} (W/mK) for 100 test samples. (shaded region includes the estimated samples with % of deviation > 10)

of samples for which the percentage of deviation exceeds 10% is more or less equal for both k_{xx} and k_{yy} (figs. 3 and 4) whereas, for k_{zz} nearly 15 samples exceeds 10% deviation (figs. 5). Though the deviation from the actual value for some samples are greater than 10%, the confidence internal encloses the actual parameter value for all parameters for all test samples. The estimation of parameters for samples falling in the interval 0.1≤ k_{xx} ≤0.5, 0.1≤ k_{yy} ≤0.35 and 0.1≤ k_{zz} ≤0.7, is observed to frequently exceed 10% of deviation from the actual value.

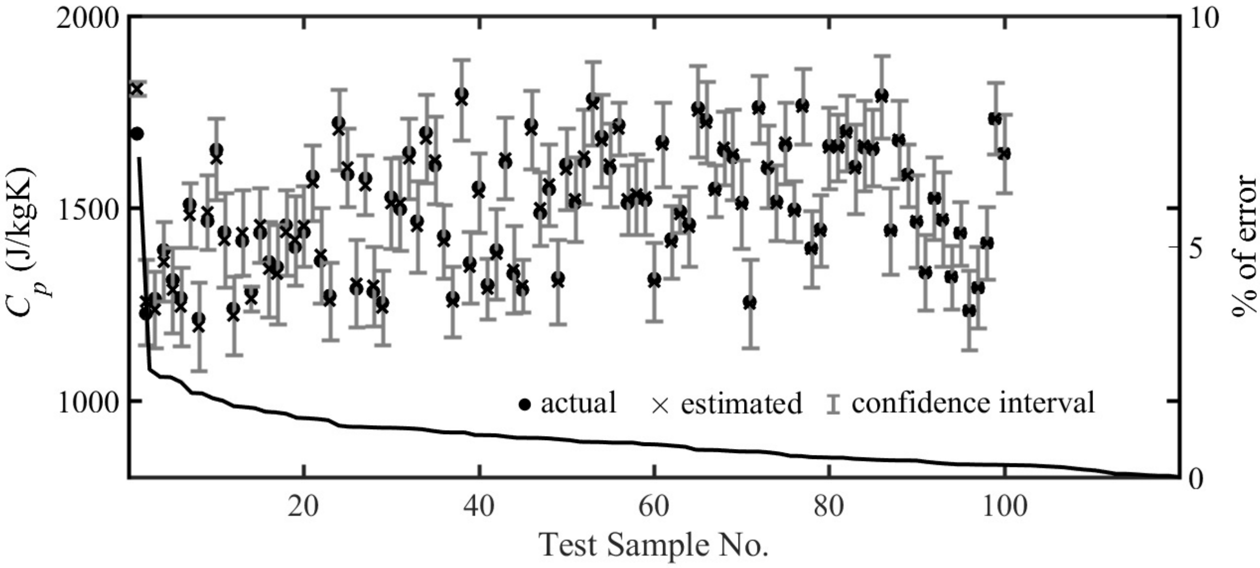

Figure 6. Estimated C_p (J/kgK) for 100 test samples.

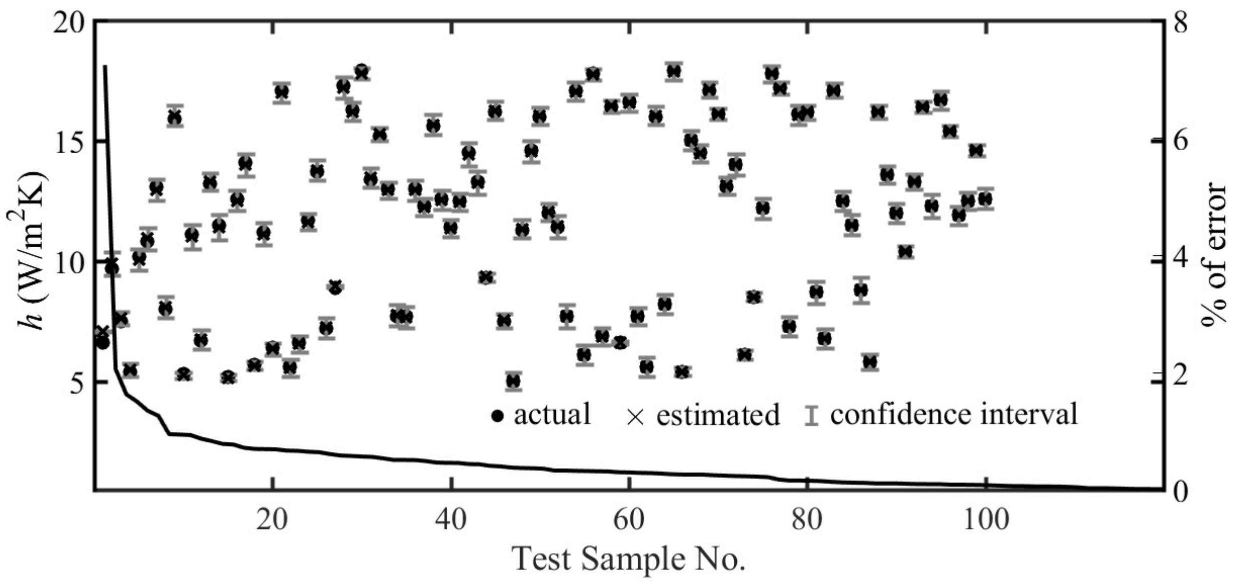

Figure 7. Estimated h (W/m^{2}K) for 100 test samples.

Therefore, one combination of parameters[4], that falls in this interval is again estimated, but using Levenberg-Marquardt algorithm with same set of experimental parameters (t, t_f, q, number of sensors). From this numerical study, it is found that the percentage of deviation for k_{xx}, k_{yy} and k_{zz} is greater than 10% even with deterministic search[5], indicating that the sensitivity of these properties with respect to experimental parameters are less and with the presence of random temperature measurement error, the inverse problem becomes more ill-posed leading to erroneous solution. Therefore, in conclusion deciding the optimum choice of experimental parameters

[4] k_{xx}=0.474W/mK, k_{yy}=0.162W/mK, k_{zz}=0.434W/mK, C_p=1693J/kgK, h=6.6W/m^{2}K
[5] however, if the initial guess is close to the actual parameter, then the percentage of deviation is $< 10\%$

for desired range of unknown parameters may reduce the estimation error. Alternatively, the present GPR trained surrogate forward model can be effectively used for estimating thermal properties falling in the range 0.5$\leq k_{xx} \leq$10W/mK, 0.35$\leq k_{yy} \leq$2W/mK, 0.7 $\leq k_{zz} \leq$2W/mK, 1200$\leq C_p \leq$1800J/kgK and 5$\leq h \leq$18W/m^{2}K.

In the present work, the effect of parameters of the covariance function (signal standard deviation and length scale) on parameter estimation are not studied while training the data. Therefore, there is scope for the future work to optimize these parameters. Also, constant length scale is used in the present work for training such large data, whereas in the future different length scales may be used for training large data sets which significantly reduce the computational effort required for training.

5. Conclusion

In this work, an inverse heat conduction problem was solved using surrogate forward model (data-fit model). A supervised machine learning process-Gaussian Process Regression (GPR) was used to construct the surrogate forward model from the simulated input and output data. The thermal properties of orthotropic materials were estimated simultaneously using the trained surrogate model. The robustness of the model in estimating the parameters was studied by carrying out the estimation for 100 new test samples and it was found that the Mean Percentage Deviation were less than 10% for all parameters. However, the percentage of deviation for some samples of parameters in the range 0.1$\leq k_{xx} \leq$0.5, 0.1$\leq k_{yy} \leq$0.35 and 0.1$\leq k_{zz} \leq$0.7 were more than 10% and it was found that, by proper choice of experimental parameters, this estimation error could be reduced while estimating the parameters in this range. Alternatively, the present GPR trained surrogate forward model could be effectively used for estimating thermal properties falling in the ranges of 0.5$\leq k_{xx} \leq$10 W/mK, 0.35$\leq k_{yy} \leq$2 W/mK, 0.7 $\leq k_{zz} \leq$2 W/mK, 1200$\leq C_p \leq$1800 J/kgK and 5$\leq h \leq$18 W/m^{2}K thus enabling to estimate wide range of thermal properties of orthotropic materials.

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