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Numerical identification of a linear oscillator stiffness using Bayesian inference and Markov chain Monte Carlo

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Abstract: Inverse problem techniques have been used in different engineering application aiming to convert observed measurements or data acquired together to the prior knowledge of the system into information about material properties, geometry, locations of anomalies, e.g. cracks and structural damage, excitation force, among others. The present papers aim to estimate parameters of a dynamic system with the inverse problem using Bayesian Inference technique. Multiples studies are presented to analyse the statistical significance of the catches for the settings, making a critical analysis between a solution via Bayesian Inference linked to minimising the objective function with stochastic methods. It applied through stochastic strategies as the Maximum Likelihood (MLE), Least Squares (LSE) and Markov Chains Monte Carlo (MCMC), implemented with the Metropolis-Hastings algorithm (MH). In the estimation, the random parameters assumed distribution inference of Gaussian and Uniform types for different standard deviations. The results demonstrated the efficacy of Bayesian inference to estimates parameter of the oscillator systems from its dynamic response and the statistical parameter information.

Keywords: Bayesian Inference; Maximum Likelihood; Markov Chain Monte Carlo (MCMC); Inverse problem; Parameters estimation; Dynamic system.

1. Introduction

There is a growing demand for more realistic system analyses covering structures from all engineering sector. There is an increasing availability of highly accurate measuring tools suitable for the most varied types of mechanical systems. In this context, several scientific challenges arise with a focus on the construction of computational models and development of algorithms (Hatch, 2001), which considers both the current state of the structure and the uncertainties associated to the system. An inverse problem basically is as a general structure that converts the observed measures and prior knowledge into information about a physical system. In this context, a wide field of research stands out aiming to develop techniques to estimate parameters, calibrate the numerical models, and quantify the system uncertainties. The scientific challenges are gaining visibility due to the growing popularity of intelligent data exploration methods and the computational techniques available to solve them (Rouchier, 2018).

The inverse problem theory offers a framework for solving parameter estimation and model calibration desirable. Several types of estimators are described in the literature. Widespread probabilistic methodologies that allow estimating the value of a set of parameters based on measurements observed for inference on inverse problems are the Maximum Likelihood, Least Squares and the MCMC. In the Bayesian approach, the inverse problem is reformulated into a search for information using statistical tools. The purpose of Bayesian Inference is to report all available information about a problem, with information from the observed data, through probabilistic statements through Bayes' Theorem (Mohammad-Djafar, 1998; Albuquerque,2018). In this method, all parameters and measurements are considered random variables, with the uncertainties associated with the variables described by a probability density function (*PDF*)(Dashti and Stuart, 2016). Castello and Ritto (2015) in their book, presented an introduction about stochastic modelling, quantification of uncertainties applied to parameters estimation via Bayesian



Inference. Fox (2010) published a book covering a complete treatment of Bayesian response modelling applied in a variety of applications.

The Maximum Likelihood Estimation (MLE), a method to estimate the parameters of a given *posterior PDF*, maximises observed data from the *prior PDF*, which follow a given distribution (Myung, 2003). Kaipio and Somersalo (2006) presented in their textbook basic and classic concepts of inverse problems such as Maximum Likelihood estimation and the Conjugate Gradient method. Oliveira et al. (2018) performed the parameter estimation by the MCMC, as well as the Maximum Likelihood approach. The Least Squares (LSE) does not require maximum or minimum distributive assumptions, it is useful to obtain a descriptive measure to minimise observed data, but there is no possibility to build confidence intervals of the analysis. The LSE estimator can be independent according to the type of noise probability distribution. Song et al. (2018) proposed a methodology for Bayesian model updating model for systems with geometric singularities based on their normal nonlinear modes extracted from broadband vibration data. The estimation was performed by the LSE and the Monte Carlo transitional Markov chain.

One of the methods applied associated with the Bayesian strategy is the Monte Carlo via Markov chain (MCMC). The MCMC algorithms provide flexible and robust solutions for estimating the later probability density. From this technique, it is possible to generate a high-dimensional *posterior PDF*, without the need to do a high-dimension integration to calculate the normalisation constant of the distribution (Jin et al.,2019). There are several methods in the literature to improve the efficiency of the estimators resulting from the MCMC, among which the Metropolis-Hastings (MH), Adaptive Metropolis algorithm (AM) (Haario,2006), Hamiltonian Monte Carlo (Green, 2015) and the Delayed Rejection method (DR) (Green,2015; Haario,2006). Vrugt (2016) described a basic theory review of Monte Carlo simulation of the Markov chain and Differential Evolution Adaptive Metropolis (DREAM) algorithm. Besag et al. (1995) performed the basic MCMC methodology, emphasising the Bayesian paradigm, conditional probability and the intimate relationship with Markov's random fields in spatial statistics. Dahlin (2015) provided an introduction to the Metropolis-Hastings (MH) algorithm for parameter inference in nonlinear state-space models together with software implementation in the statistical programming R language. Khalil et al. (2015) studied a nonlinear inverse problem displaying a noisy disturbance to estimate time-invariant parameters via MCMC.

The present work aims to demonstrate how to use the theory of inverse problems based on the Bayesian inference combined with the MLE, LSE and MCMC-MH to estimate the stiffness of the oscillator systems from its dynamic response, and the statistical parameter information. The mathematical formulation of the oscillator physical problem is developed under the framework a single degree of freedom composed by a mass-spring-damper. The direct problem is solved analytically, and the obtained resonance frequency used as an input system response information in the inverse problem procedure.

2. Inverse problem

All parameters and measurements are considered random variables in an inverse problem via a Bayesian approach, and the uncertainties associated with these variables are described by a chosen *PDF* (Kaipio and Somersalo, 2006). The objective of the method is to extract information and evaluate uncertainties about the variables based on the available knowledge of the measurement process, as well as data and models of the unknowns variables before the measurement process.

2.1. Bayesian Inference

The process of building up a given computational model (\mathcal{M}) is considered to describe the physical system (\mathcal{B}) . Also, a set of measurements (y) is known, and the structuring process will take place from the identification of the parameters vector of interest (θ) . The y and θ are random variables, so the model response is given by $y^m = y^m(\theta)$. The *posterior* probability distribution function, which relates the *PDF*s of the experimental data to the vector of parameters of interest $\pi(\theta|y)$, which follows the Bayes theorem expressed in terms of probability distributions takes the form (Lynch 2008)

$$\pi(\theta | y) = \frac{\pi(y | \theta) \pi(\theta)}{\pi(y)}$$
(1)

where $\pi(y|\theta)$ represents the system's likelihood function, $\pi(\theta)$ prior probability density function, and $\pi(y)$ the probability density function associated with the experimental data, the information about the likelihood *PDF* can be

obtained by using a particular model of observation of the system. By considering the relationship between the observed data (y) and the predictions of the model $(y(\theta)^m)$, it can be described from an observation model with additive error (v) as follows

$$y^{exp} = y(\theta)^m + \nu, \tag{2}$$

where the ν is an additive noise that describes the difference between experimental observation and the prediction of the model, represented by a random vector, therefore, given that y, θ , and, ν are random variables will be related to a joint *PDF* $\pi(y, \theta, \nu)$ (Castello and Ritto, 2015). By considering that the noise is stationary, Gaussian with known variance σ_{ν}^2 , the likelihood function can be represented by

$$\pi(y^{exp}|\theta_i) = \frac{1}{(2\pi)^{n/2}\sigma_v^n} exp\left(-\frac{1}{2} \frac{\left(y^{exp} - y^m(\theta_i)\right)^T \left(y^{exp} - y^m(\theta_i)\right)}{\sigma_v^2}\right).$$
(3)

The likelihood *PDF*, $\pi(y^{exp}|\theta_i)$, corresponds to the probability of having measured data y^{exp} given a specific model $y(\theta)^m$, defined by the parameter set θ . To obtain information about the unknown parameters may be obtained via Statistical Inversion Theory or other techniques as the Maximum Likelihood (MLE) and Least Squares Estimation (LSE).

2.2. Maximum Likelihood and Least Squares Estimation

To determine the target estimator of the parameter of interest $\hat{\theta}$, the expected value of the *posterior* PDF expressed by

$$\hat{\theta} = \int \mathbf{m}k \,\pi(\theta | y^{exp}) dk. \tag{4}$$

The estimator that results aim the maximum value of the likelihood is denominated Maximum Likelihood Estimator (MLE), $\hat{\theta}_{MAX}$. For a problem with Gaussian additive noise and *prior* uniform *PDF* for the parameter of interest, the MLE will have the same numerical result as that of Least Squares (Oliveira et al. 2018). Therefore, the MLE is defined as

$$\hat{\theta}_{MAX} = \arg\max_{\theta} \pi(y^{exp}|\theta) \tag{5}$$

The Least Squares Estimator (LSE) assumed the residual rule of the $||r = y^{exp} - [U]\theta||$ the system, which can be obtained by

$$\hat{\theta}_{MIN} = \arg \min_{\theta} \|y^{exp} - [U]\theta\|^2 \tag{6}$$

2.3. Markov Chain Monte Carlo Metropolis-Hastings algorithm

Markov chain Monte Carlo (MCMC) develops sequences that converge from a distribution to a target, in this case, the *posterior* distribution. Then, the mean value of the sample is calculated to obtain the best value inferred from the *posterior PDF*. The MCMC methods are conceptually simple, and the algorithms are easy to be represented (Albuquerque et al., 2018). Any method capable of producing samples $\{\theta^{(1)}, \dots, \theta^{(N)}\}$ and has a stationary probability distribution of $\pi(\theta)$ is considered a Monte Carlo method via the Markov chain for a simulation of a probability density distribution. The main feature of this technique is that the samples are performed sequentially so that the distribution of the j-th sample, $\theta^{(j)}$ depends on the previous sample, $\theta^{(j-1)}$ with the course of iterations.

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2.3.1. Metropolis-Hastings algorithm

The Metropolis-Hastings (MH) algorithm is a common technique for sampling the *posterior PDF* created from the MCMC (Green and Worden, 2015). There are other types of algorithms, e.g. Adaptative Metropolis, Hamiltonian Monte Carlo and Hybrid Monte Carlo, which aim to obtain a sequence of random samples from a probabilistic distribution for the which direct sampling are complex. The algorithm works by starting with the likelihood function in each Markov chain is proposed a sample candidate with *j*-repetitions evaluated of the iteration $\theta^{(c)}$ and its predecessor $\theta^{(j-1)}$ as follows:

$$\alpha(\theta^{(c)}, \theta^{(j-1)}) = \frac{\text{posterior of } \theta^{(c)}}{\text{posterior of } \theta^{(j-1)}}$$
(7)

The transition function will be a Gaussian distribution centred on θ associated with the standard deviation σ_{exp} , such as $\theta^{(c)} \sim N(\theta^{(j-1)}, \sigma_{exp})$. By considering the symmetry of this distribution, the probability of acceptance is reduced to the ratio between the generated *posterior PDFs* and does not depend on the transition density function. Thus, the new probability value in the $\theta^{(c)}$ acceptance process proposed by the MH algorithm with a related Gaussian transition function can be described as (Kaipio and Somersalo, 2006):

$$\alpha = \min\left[1, \frac{\pi(\theta^{(c)}|y^{exp})}{\pi(\theta^{(j)}|y^{exp})}\right].$$
(8)

3. Single degree of freedom oscillator dynamic system

This section presents a brief formulation of the dynamic oscillator analysed in this paper. The mechanical vibration of structures with a single degree of freedom is considered the simplest case to describe the movement of a system subject to some initial condition. These are ideal systems, capable of representing a small part of the existing real systems. On the other hand, systems with a single degree of freedom have characteristics that support the understanding of most of the fundamental aspects existent in more complex systems. The purpose of physical modelling is to represent all the important aspects existing in the system for the determination of the mathematical equations of motion of the system. Figure 1 presents a schematic drawing of the physical model used for the next studies. It is a linear oscillator composed of an inertial, elastic element and a dissipating element.



Figure 1. Linear single degree of freedom oscillator system composed by a mass-spring-damper.

The governing equation of motion expressed in equation (9), obtained from the forces acting on the specimen, is described by an ordinary differential equation with constant coefficients that relates the displacement, u(t) and the acting force, F(t). Therefore, the dynamical system equation of motion is given as

$$m\ddot{u}(t) + c\dot{u}(t) + ku(t) = F(t), \tag{9}$$

where, $\ddot{u}(t) = d^2 u/dt^2$ is the mass (m) acceleration and $\dot{u} = du/dt$ the velocity (Meirovitch, 2000), m is the mass, c the damper, and k the spring. It is also a common practice to work in terms of the system's descriptive coefficients. By dividing the equation (9) by the mass (m), we obtain the relation

$$\ddot{u} + 2\xi\omega_n\dot{u} + \omega_n^2 x = f(t),\tag{10}$$

where ω_n is the natural frequency defined by relating the mass to the spring as $\omega_n = \sqrt{k/m}$, and damping coefficient (ξ) expressed as $\xi = c/2\omega_n m$. The dynamic mechanical systems are also considered for the free vibration case when the dissipative element in not take into account. Therefore, to obtain the time response of a system subject to an initial condition is necessary to solve the simplified homogeneous ordinary differential equation that describes the movement, given by:

$$m\ddot{u}(t) + ku(t) = 0; \quad or \quad \ddot{u}(t) + \omega_n^2 u(t).$$
 (11)

and the natural frequency is also obtained as $\omega_n = \sqrt{k/m}$.

4. Numerical results

To verify the methodology, the spring-stiffness parameter of the mechanical oscillator systems is estimated, and some simulation results presented in this section. The Bayesian Inference method is applied to formulate the problem, and the Maximum Likelihood (MLE), Least Squares (LSE) and Markov chain Monte Carlo (MCMC) used to optimise the estimation. MCMC-HM has been implemented in MATLAB, and the MCMC of the UQLAB toolbox used in the estimation process (Lataniotis, Marelli, and Sudret 2019). The oscillator stiffness (k) is regarded as unknown, and will be estimated from the synthetic measured force and resonance frequency ω_n^{exp} . In the following problem, equation 12 is the object of study to estimate the stiffness. It is noteworthy that the data sample is generated randomly following Gaussian probability distribution. By considering an additive error ν with Gaussian distribution so that the relationship between the observed data $(\omega_n^{(exp)})$ and the predictions of the model $(\omega_n = \sqrt{k/m})$, the ressoannce frequency can be described as

$$\omega_n^{exp} = \sqrt{\frac{k}{m}} + \nu, \tag{12}$$

for ω_n^{exp} , k is assumed as random variables. Those variable associated with their probabilities distribution when correlated generates a joint *PDF*, $\pi(\omega_n, k)$, as

$$\pi(\omega_n|k) = \int \pi(\omega_n|k,\nu) \ \pi(\nu|k) \ d\nu , \qquad (13)$$

for $\nu \in \mathbb{R}^n$ such that $\nu \sim \mathcal{N}(0, \Sigma_{\nu})$. Since it is an appropriate approximation of the covariance matrix associated with errors, $\Sigma_{\nu} = \sigma_{\nu}^2 I_{nxn}$. Therefore, the likelihood equation is expressed by

$$\pi(\omega_n|k) = \frac{1}{(2\pi)^{n/2}\sigma_v^n} exp\left(\frac{-1}{2} \frac{\left(\omega_n^{(exp)} - \left[\sqrt{k/m}\right]\right)^T \left(\omega_n^{(exp)} - \left[\sqrt{k/m}\right]\right)}{\sigma_v^2}\right).$$
 (14)

The posterior PDF is related to the likelihood function defined in Eq. (14) with the prior assumed as uniform distribution in a limit between 1 to 30, $k \sim \text{UNIF}(1,30)$. In this analysis, we considered as a reference value for the stiffness equal to $k^{ref} = 15 \text{ N} / \text{m}$. Two sets of observations $\{\omega_1^{exp}, \omega_2^{exp}\}$ have been generated and were used to parameter identification. The two sets of data were carried out to verify the change in the estimation results for different sets of samples (Kruschke, 2010).

4.1.1. Estimation via Least Square and Maximum Likelihood

Figure 2 presents the estimation results obtained with the MLE in figure 2(a) and LSE in figure 2(c). Each *posterior* sample parameters were generated by multiply the likelihood and the *prior* and stiffness evaluated by the calculation of the *posterior* function maximum value. And by the *posterior* function minimum value in the case of LSE. The graphic in figure 2(a) shows the *PDFs a posteriori* of the data sets generated close to the reference value (k^{ref}). For both sets of samples, the resulting functions were close to the stiffness reference number. Figure 2(b) is the error function in logarithmic scale, which displays the likelihood on a logarithmic scale versus the function of the error norm (*r*). It presented a descending line whose maximum point goes to zero.



Figure 2: MVE results: (a) *Priori* and *posterior* probability density functions and the reference value for constant stiffness analysis for two sets of experimental data $\{\omega_{n1}^{exp}, \omega_{n2}^{exp}\}$; (b) Logarithmic scale analysis of the residual function norm; (c) Residue function and likelihood function for each method.

Figure 2(c) shows the likelihood functions and least-squares ($\|\omega_n^{exp} - \sqrt{k/m}\|^2$) for the two sets of observations. It is clear that the maximum and minimum points of the dashed and continuous graphs, in blue and black, again coincided, thus demonstrating the theory regarding the Maximum Likelihood and Least Squares strategies. The arbitrary parameters used for this case study, for the two data sets, the values of ω_{n1} and ω_{n2} generated by the computational model, together with the results estimated by the MLE and LSE, are shown in Table 1.

Table 1. Observed results for Maximum Likelihood and Least Squares methods σ_{exp} = 5 %.

	ω_n^{med} [rad/s]	ω_{n1}^{med} [rad/s]	ω_{n2}^{med} [rad/s]	Mass [kg]	$\widehat{k}_{MAX}[{ m N/m}]$	\widehat{k}_{MIN} [N/m]
1 st set	1.963	0.113	0.185	1	14.18	14.18
2 nd set	3.873	1.696	1.951	4	16.23	16.23

The results obtained by the Maximum Likelihood and Least Squares strategies were coincident. The reference value for stiffness was 15 N/m. Because of this, it was possible to corroborate the correct application of these methods, since they satisfied the theory of equality between the estimated points for the asymmetric distribution of probabilities of the function *a posteriori*.

4.1.2. Estimation via MCMC-MH

Next, the estimation of equivalent stiffness of the system from ω_n^{exp} as input will be solved by Markov Chain Monte Carlo – Metropolis-Hastings (MCMC-MH) algorithm. Equation (15) represents the numerical model used to generate the sample points and possible candidates in the Markov chain to generate the *posterior PDF*. It was assumed a variability of $\sigma_{exp} = 5 \$ bias on Gaussian distribution. Therefore, the probability of acceptance of a new candidate for the rigidity of the system $(k^{(c)})$ occurs from the application of the MH algorithm, so that the probability of acceptance of possible candidates $(k^{(c)})$ in the chain with a current status (j) can be described as follows

$$\alpha(k^{(c)}|k^{(j-1)}) = \frac{\pi(k^{(c)}|\omega_n^{exp})}{\pi(k^{(c-1)}|\omega_n^{exp})}$$
(15)

Figure 3(a) shows the evolution of the chain generated by MCMC-MH of the *posterior PDF* for 10000 iterations, the reference value, and the estimated stiffness. There is a stationary trend in the simulations created around the estimation point over the Monte Carlo (MC) iterations (Christen, J Andrés and Fox, 2005). It demonstrates that *posterior PDF* provides a mean value associated with a standard deviation. Besides, figure 3(b) shows the histogram of the probability density corresponding to the generated chain. A good symmetry in the histogram was achieved, which allowed a Gaussian adjustment and a heuristic convergence indicator leads to the stiffness estimation.



Figure 3: Bayesian Inference Results via MCMC-MH: (a) *a posteriori* generated by MCMC, a reference value and the expected value of the stiffness; (b) histogram of the probability density, with a Gaussian fitting distribution for *k* values

A summary of the pre-processing conditions of the input data and the results obtained by MCMC-MH algorithm are presented in Table 2. The results presented in Tables 1 and 2 demonstrate that, for the same variance σ_{exp} assumed in the MLE and LSE techniques, the point result obtained by MCMC-MH for stiffness was the closest to the reference value.

Table 2. MCMC- MH estimation result for an error of	$\sigma_{exp} = 5$	\%
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Prior PDF	σ_{exp}	MCMC iterations	k_{ref} [N/m]	k_{est} [N/m]	
Gaussian	5%	10000	15	13.99	

4.1.3. Estimation using MCMC UQLab toolbox

The use of the MATLAB-UQLab toolbox aimed to improve the MCMC estimation algorithm. The sampling points obtained from a Gaussian probability distribution, and six random sampling points generated from the computational model with an associated additive error (Eq. 15). The parameter of interest was assigned as a Log-Normal distribution (Schevenels, Lombaert, and Degrande, 2004) with a mean value centred on the reference point. The standard deviation σ_{exp} , was considered unknown and, as initial information, a Uniform distribution is imposed, so that $\sigma_{exp} \sim \text{UNIF} (0, 0.5)$. Figure 4 shows the evolution of the MCMC chain and its respective Kernel density.



Figure 4. trace graph and corresponding KDE during the execution of the MCMC-MH

The generated MCMC immediately converged to the stiffness reference value. The Kernel graph that Kernel density (KDE) is well defined, with a symmetrical curve as a Gaussian probability distribution, which indicates a good convergence of the MCMC to the estimated value. Figure 5 (a-b) presents the predictive *prior* and *posterior* distributions estimated with the MCMC chain generated sample data and the histograms with of the mean point. The undefined σ_{exp} was estimated from the experimental data, whose prior information of the error components previews defined.



Figure 5. Histograms of the *prior* and *posterior* predictive distributions with the empirical mean $E[k|y_{exp}]$ estimated from the MCMC sample data and dispersion graphs of the prior and posterior samples: (a) Histograms *prior* to the sampling points; (b) Histograms *a posteriori* of the sampling points

From the histograms of figure 5(a), on top it is the initial Log-Normal distribution attributed to the parameter k, the sample cloud followed by a uniform *prior* distribution from 0 to 0.5 associated with σ_{exp} . Figure 5(b) shows how the candidates behaved in the generation of the *posterior* distribution of the stiffness with the *prior* distribution. The mean values points for both parameters k and σ_{exp} are represented in red.



Figure 6. Variation of the expected value of the stiffness to 10.000 iterations.

Convergence graphic showed in Figure 6 demonstrated that around 2500 step up a good stabilisation of the parameter estimation close to the stiffness reference value. It indicates that the number of iterations adopted was sufficient to obtain a good convergence of the results. Table 3 presents the estimated results by using the UQLab toolbox compared to the reference value.

Table 3. MCMC- UQLab estimation result using ω_n data

Parameter	k_{ref} [N/m]	k_{est} [N/m]
k	15	15
σ_{exp}	-	0.24

By comparing the MCMC obtained using the toolbox, with those results obtained with MCMC-MH, Table 2, a considerable improvement in the parameter was achieved by using the UQLab. It because UQLab toolbox(Lataniotis, Marelli, and Sudret **2019**) run a few simultaneous chains at the same time, which improves the estimation performance. While the MCMC-MH implemented code used a single chain each time in the estimation procedure. However, both techniques aim the MCMC-MH algorithm presented in section 2.

5. Conclusions

The analysis of inverse problems using stochastic strategies has proved to be an efficient tool to obtain accurate information about models in different areas of knowledge. This papers sought to apply the Maximum Likelihood (MLE) and Least Squares (LSE) estimators, with a focus on Bayesian inference in mechanical systems, where initial data about the problem was known and demonstrates an overview of the steps and tools to explore the target information from the experimental data. The use of MCMC-MH it was possible to obtain results from the *posterior PDF*. The UQLab Bayesian inference toolbox was used to evaluate the estimation. The results obtained with MLE, LS and MCMC performed an excellent estimation. However, the MCMC and MCMC-UQLab were the best methodologies to run the optimisation process.

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