CZECH TECHNICAL UNIVERSITY IN PRAGUE
FACULTY OF CIVIL ENGINEERING
DEPARTMENT OF MECHANICS

IDENTIFICATION OF ALEATORY UNCERTAINTY IN PARAMETERS OF HETEROGENEOUS MATERIALS

Doctoral thesis statement

Ing. Eliška Janouchová

Doctoral Degree Program: Civil Engineering
Branch of Study: Physical and Material Engineering

Supervisor: Ing. Anna Kučerová, Ph.D.

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ABSTRACT

Advances in meta-modelling and increasing computational capacity of modern computers permitted many researches to focus on parameter identification in probabilistic setting. Parameter identification of a heterogeneous material model can be formulated as a search for probabilistic description of its parameters providing the distribution of the model response corresponding to the distribution of the observed data , i.e. a stochastic inversion problem.

This topic is addressed by only few works available in the up-to-date literature, each having some relevant limitations. In the present, the estimation of aleatory uncertainties is often connected to Bayesian inference based on hierarchical modelling when some specific shape of probability density function of the model parameters is assumed. Another identification method uses optimal maps based on optimisation of a transformation function between prior and posterior distributions. The approach allows to relax the assumptions about the specific form of the parameters' distribution, but actually it is developed only for quantification of epistemic uncertainties. The goal of the doctoral thesis is to review, compare and extend the available methods for identification of inherent variability (aleatory uncertainties) with application in calibrating heterogeneous material models.

Keywords: stochastic inversion problem, stochastic modelling, aleatory uncertainty, polynomial chaos expansion, principal component analysis, transformation of random variables, Bayesian identification, Markov chain Monte Carlo sampling, heterogeneous materials

ABSTRAKT

Díky vývoji metamodelů a vzrůstajícímu výkonu výpočetní techniky se mnozí výzkumníci mohou zaměřit na pravděpodobnostní přístupy k identifikaci parametrů. Identifikaci parametrů modelu heterogenního materiálu lze formulovat jako hledání pravděpodobnostního popisu jeho parametrů poskytující rozdělení odezvy modelu, které koresponduje s rozdělením naměřených dat, tj. stochastický inverzní problém.

Tímto tématem se zabývá pouze několik prací dostupných v současné literatuře, kdy každá má určitá omezení. V současnosti je odhad aleatorických nejistot často spojován s bayesovskou inferencí založenou na hierarchickém modelování, kdy se předpokládá určitý tvar funkce hustoty pravděpodobnosti parametrů modelu. Jiná identifikační metoda používá optimální mapy založené na optimalizaci transformační funkce mezi apriorním a posteriorním rozdělením. Tento postup sice umožňuje upustit od předpokladu konkrétní podoby rozdělení parametrů, ale je vyvinut pouze pro kvantifikaci epistemických nejistot. Cílem disertační práce je prozkoumat, porovnat a rozšířit dostupné metody pro identifikaci přirozené variability (aleatorických nejistot) s aplikací v kalibraci modelů heterogenních materiálů.

Klíčová slova: stochastický inverzní problém, stochastické modelování, aleatorická nejistota, polynomiální chaos, analýza hlavních komponent, transformace náhodných proměnných, bayesovská identifikace, Monte Carlo pro Markovovy řetězce, heterogenní materiály

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CHAPTER 1

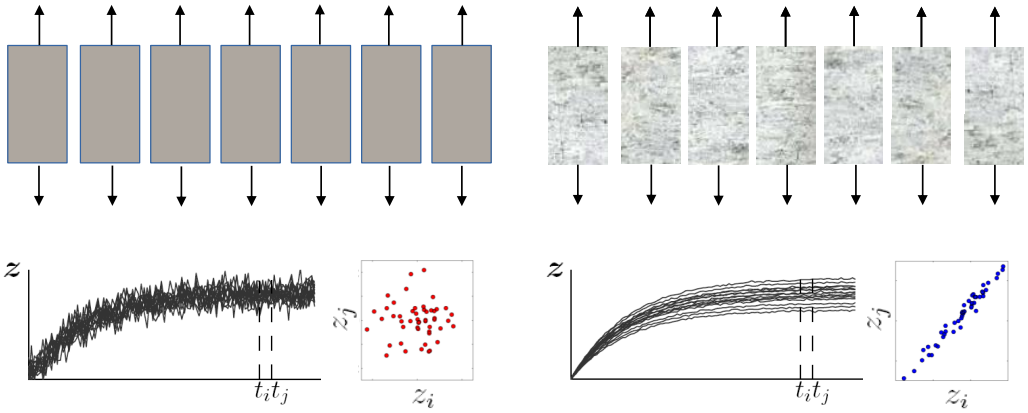
INTRODUCTION

In order to predict the behaviour of the structural system under the loading in a computational way, the corresponding numerical model has to be properly calibrated. In other words, parameters of the mathematical model of the system have to be estimated as accurately as possible to obtain realistic predictions, e.g. for usage in an appropriate reliability analysis or structural design optimisation.

Heterogeneous character of building materials causes spatial variations of mechanical parameters (such as elastic modulus, yield stress or tensile strength) affecting the structural system behaviour under the loading. This phenomenon can be best observed during the laboratory tests on a set of specimens made of the same heterogeneous material. Differences in morphology of individual specimens induce a significant variability in observed values, c.f. Fig. 1.1b. To this end, two main approaches were developed within the last decade. The first one focuses on material morphology at a micro-level and propagates the uncertainty to the macro scale using the techniques of stochastic homogenisation [63, 3, 26]. The second approach, principally different, aims at identifying the uncertainty in material parameters indirectly from macroscopic observations of a structural response by solving a stochastic inverse problem. Stochastic inversion searches for a probabilistic description of stochastic model parameters providing the distribution of the model response corresponding to the distribution of the observed data.

In this context, uncertainties can be divided into two main categories according to whether a source of nondeterminism is irreducible or reducible [43]. Our goal is to quantify aleatory (irreducible, inherent, stochastic) uncertainty which corresponds to real variability of properties in the heterogeneous material, while epistemic (reducible, subjective, cognitive) uncertainty arising from our lack of knowledge is supposed to be reduced by any new measurement according to the coherence of learning [34, 8]. Difference between two types of uncertainties with respect to material properties are illustrated in Fig. 1.1.

Inverse problems are often ill-posed, because the function mapping the parameters to the



$z(t) = y(\boldsymbol{x}) + \varepsilon(\omega)$ (a)

$z(t) = y(\boldsymbol{x}(\theta)) + \varepsilon(\omega)$ (b)

Figure 1.1: Fundamental difference between homogeneous (a) and heterogeneous materials (b), respective epistemic uncertainty and combination of epistemic and aleatory uncertainty.

responses is not injective so it is also non-invertible. The most common method of parameter estimation is based on fitting the response of a model to the experimental data. This approach leads to optimising parameters so as to minimise the difference between the data and the model response. On the other side, in the last decades probabilistic methods to stochastic modelling of uncertainties have became applicable thanks to a growing computational capacity of modern computers. An extensive overview on stochastic modelling of uncertainties can be found in [54]. The probabilistic approach restates the inverse problem as well-posed in an expanded stochastic space by modelling the parameters as well as the observations as random variables with their probability distributions [32]. Several methods for the uncertainty quantification in probabilistic settings have been proposed in the literature.

The last decade witnessed an intense development in the field of Bayesian updating of epistemic uncertainty in description of deterministic material or structural parameters, see e.g. [36]. Here, a likelihood function is established to quantify our confidence in observed data, with the goal to update our prior knowledge on material properties [50]. The increasing popularity of Bayesian methods is motivated by developments in the field of spectral stochastic finite element method, which allows to alleviate the computational burden by surrogate models such as polynomial chaos expansions (PC) [35]. We wish to emphasize that this approach is designed only to the epistemic uncertainties, see Fig. 1.2a, by its applications to heterogeneous materials provides us with the mean values and a small range of uncertainty which shrinks with additional measurements, c.f. Fig. 1.2b.

Quantification of aleatory uncertainties (see Fig. 1.2c) in parameters of a nonlinear physical model is significantly less elaborated. One of the identification approaches is based on choosing a particular type of probability density function (PDF) of the identified aleatory quantities and the corresponding moments of this statistical model are provided by e.g. maximum likelihood method (MLE) or perturbation method [20]. The proposed methods

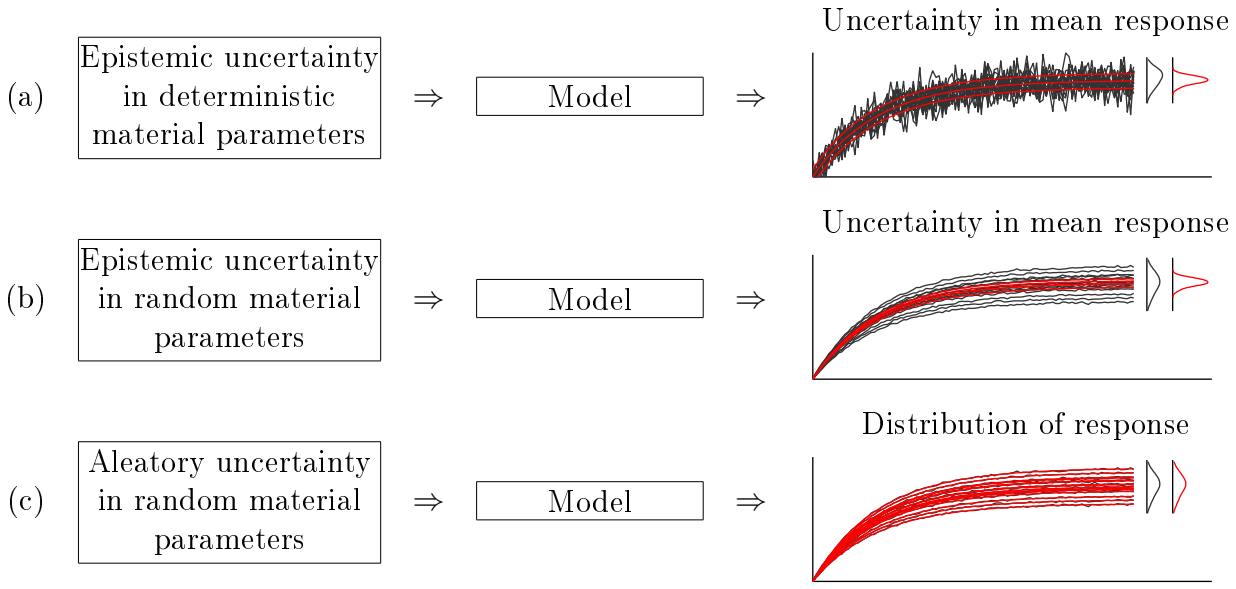


Figure 1.2: Scheme of an experiment and different approaches to parameter identification

have several crucial limitations. First, the assumption of a known type of a statistical model is very limiting and prohibits the identification of higher statistical moments. The perturbation method (even when extended by other nonlinear terms) is hardly applicable to nonlinear models and Monte Carlo-based MLE faces high computational requirements. Recently, authors in [19] and [53] employed independently PC-based surrogates to accelerate the identification of aleatory uncertainties formulated as a deterministic optimisation problem. In particular, statistical moments or PC coefficients defining the statistical model of physical parameters are optimised so as to fit the corresponding moments of the model response to the moments obtained from the experiments. While [19] emphasizes that the PC-based surrogate of a model response provides an efficient way for computing sensitivities, [53] focuses on PC ability to effectively represent higher statistical moments and identify non-Gaussian parameters. Nevertheless, many related issues remain unsolved. For instance, quantification of related epistemic uncertainties is not considered at all. It means that the methodology is not able to reflect the number and the value of additional measurements. Also the application of the proposed methods to the set of correlated observations, which are typically obtained by measuring e.g. load-displacement curves or by collecting the observations from a set of probes placed on each specimen can be problematic. In such a situation, the higher dimensionality of the observations leads to an increasing complexity of their joint distributions and thus to an increasing dimensionality or a number of the underlying optimisation problems.

Stochastic inversion accounting for aleatory as well as for epistemic uncertainties is addressed in several recent works [1, 40, 39, 14]. The authors employ the same methodology based on the PC-based approximation of material parameters' distribution. The PC coefficients are obtained via formulation of a likelihood function constructed for the measured data. Contrary to [20], the PC coefficients are considered here as uncertain and identi-

fied in the Bayesian way by MCMC sampling. The introduction of new random variables for describing the PC coefficients thus allows us to quantify the epistemic uncertainty in the estimated statistical model of aleatory material properties. Nevertheless, the method is derived only for a situation, where identified material parameters coincide with observed quantities. In case of measuring a response of a nonlinear physical model, a set of deterministic inverse problems is solved first, so as to estimate correlated values of spatially varying material parameters corresponding to particular spatially correlated observations. Then the obtained parameter values enter the described stochastic inversion. The inverse problem is thus divided into the solution of deterministic inverse problems and stochastic assimilation of spatially correlated estimates. Such separation is however not always feasible.

We conclude that the quantification of aleatory uncertainties is addressed by only few very recent works and requires further research, which will be the subject of the dissertation work. To be more specific, the work will be focused on combining and elaborating the aforementioned methods so as to provide methodology to (i) quantify aleatory uncertainty, (ii) reduce epistemic uncertainty with additional measurements and (iii) infer from observations described by a nonlinear model.

CHAPTER 2

BAYESIAN INFERENCE

The principal idea of the Bayesian identification is based on a common way of thought when the resulting belief about a random event is given by a combination of all available information. This approach introduces the concept of uncertainty in our subjective knowledge of the identified parameters [22, 57]. The Bayesian inference becomes increasingly popular and more widespread approach to parameter identification providing an elegant solution to this inverse problem by making it well-posed. It allows to estimate values of input parameters together with appropriate uncertainties by combining prior information and experimental measurements, see Fig. 2.1. In this case, observations are assumed to be performed for the specific yet unknown values of input parameters and epistemic uncertainty arising from experimental errors and lack of knowledge is reduced with an increasing number of experimental observations.

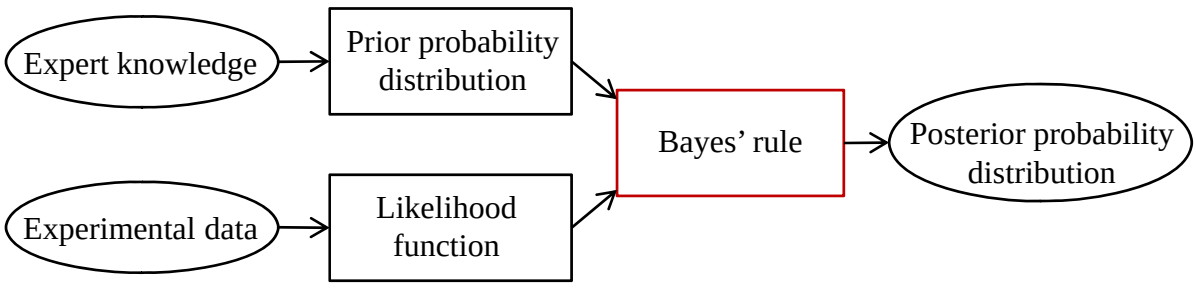


Figure 2.1: Principle of the Bayesian inference.

Consider a stochastic problem

$$\boldsymbol{z}(\boldsymbol{x}, \omega) = \boldsymbol{y}(\boldsymbol{x}) + \boldsymbol{\varepsilon}(\omega), \tag{2.1}$$

with uncertain model parameters $\boldsymbol{x}$ and random observable data $\boldsymbol{z}$, which can be predicted

by a model response $\boldsymbol{y}(\boldsymbol{x})$ besides a measurement error $\boldsymbol{\varepsilon}$. Such an identification starts with a parameters' prior distribution $p(\boldsymbol{x})$ quantifying our preliminary and typically very uncertain knowledge of parameters' value. The observations then enter through the likelihood function $p(\boldsymbol{z}|\boldsymbol{x})$ quantifying uncertainty in measurement errors. The posterior state of knowledge is obtained as the combination of the prior and likelihood resulting in posterior distribution, which contains higher amount of information and thus less uncertainty according to Bayes' rule

$$p(\boldsymbol{x}|\boldsymbol{z}) = \frac{p(\boldsymbol{z}|\boldsymbol{x})p(\boldsymbol{x})}{p(\boldsymbol{z})} = \frac{p(\boldsymbol{z}|\boldsymbol{x})p(\boldsymbol{x})}{\int_{\boldsymbol{x}} p(\boldsymbol{z}|\boldsymbol{x})p(\boldsymbol{x})\mathrm{d}\boldsymbol{x}}. \tag{2.2}$$

However the formulation of the resulting posterior probability distribution usually has a complicated formulation including the whole structural model, which cannot be treated analytically. To overcome this obstacle, several methods were developed. The most commonly referred techniques of Bayesian inference in literature are based on the Markov chain Monte Carlo method [36], less mentioned approaches utilize the Kalman filter [50] or optimal transport maps [17].

2.1 Markov chain Monte Carlo

Markov chain Monte Carlo (MCMC) is a sampling method based on a creation of an ergodic Markov chain of required stationary distribution equal to the posterior [25, 23]. There are different algorithms for constructing this chain [55], e.g. Gibbs sampler or Metropolis-Hastings algorithm, which avoids calculating of the normalisation constant in Eq. 2.2 by evaluating only ratios of target probabilities. Suitable setting of the proposal distribution for a random walk is important and can be evaluated on the basis of acceptance rate [48] or autocorrelation which is required to be minimal. The convergence speed of the procedure depends also on the appropriate choice of the starting point [23]. The essential advantage of this method is its versatility for usage with nonlinear models, when for an infinite number of samples it gives the exact solution. The disadvantage of this method is its high computational effort resulting from necessity of a high number of model simulations. In order to accelerate this sampling procedure in the identification process, the evaluations of a numerical model can be replaced by evaluations of a computationally efficient model surrogate.

2.2 Kalman filter

The second way of obtaining updated posterior distribution comprises Bayesian linear methods, see e.g. [49], based on Kalman filtering [33]. The basic idea of these methods is to update the prior random variable X_f by a linear map to a linear Bayesian posterior estimate

$$X_a = X_f + \mathbf{K}(z(x,\omega) - Y_f(X_f)), \tag{2.3}$$

where Y_f is the prior model response and the Kalman gain

$$\mathbf{K} = \mathbf{C}_{X_f Y_f}(\mathbf{C}_{Y_f} + \mathbf{C}_\varepsilon)^{-1} \tag{2.4}$$

is computed from the corresponding covariance matrices and measurement covariance C_ε.

The posterior X_a can be estimated by so called the ensemble Kalman filter algorithm based on updating of prior Monte Carlo samples, which also serve for computation of the covariance matrices. The method requires a smaller number of samples than previous MCMC method, but the identification of the uncertainty is not generally so accurate as with MCMC. Another approach is to approximate the random variables by polynomial chaos expansions, which enables to evaluate the Kalman gain and posterior X_a in an algebraic way [51]. Its main advantage is elimination of computationally demanding model simulations. However, the result is exact only in a special case of a linear model and normally distributed random variables, in another cases these methods are only approximate.

2.3 Transport maps

This technique is based on formulation of a transport function or a map which transforms the prior random variable X_f into the posterior random variable X_a [17] and arises from the context of optimal transport theory. The authors describe the map by multivariate orthogonal polynomials and the solution is obtained by the optimisation of the corresponding polynomial coefficients. The cost function is defined with a help of the Kullback-Leibler divergence expressing the discrepancy between the prior density $p(x)$ and approximate map-dependent prior density. The prior has to be expressible by standard random variables whose probability distribution is orthogonal to the chosen polynomial basis [62]. The posterior is then identified in the form of polynomial chaos expansion which is efficient in terms of analytical evaluation of posterior statistical moments. Thanks to deterministic expression of the map, one can easily sample from the posterior by transforming the prior samples.

The methodology is developed also for usage with multiscale models [45] and for accelerating MCMC [44].

CHAPTER 3

HIERARCHICAL BAYESIAN MODELLING

Bayesian approach can be extended into multilevel setting which allows to take into account also aleatory uncertainties [41, 7]. While in the classical formulation the model parameters have unknown deterministic values, hierarchical Bayesian modelling enables to consider the model parameters as stochastic variables described by some statistical model with uncertain moments. Specifically, the extension is done by introducing new random variables, known as hyperparameters $\boldsymbol{\theta}$ defining the probabilistic specification of the model parameters [22]. The parameters' prior is then conditional on the hyperparameters $\boldsymbol{\theta}$ with their own prior distribution called hyperprior $p(\boldsymbol{\theta})$, we get joint prior distribution of the parameters and hyperparameters in a form

$$p(\boldsymbol{x}, \boldsymbol{\theta}) = p(\boldsymbol{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}) \tag{3.1}$$

and according to Bayes' rule the corresponding joint posterior distribution up to a normalisation constant is

$$p(\boldsymbol{x}, \boldsymbol{\theta}|\boldsymbol{z}) \propto p(\boldsymbol{z}|\boldsymbol{x}, \boldsymbol{\theta})p(\boldsymbol{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}). \tag{3.2}$$

More specifically now we have n observations $\boldsymbol{z}_i$, each of them is realized for n combinations of input values $\boldsymbol{x}_i$ drawn from unknown distribution. Each of these combinations is defined by its prior distribution $f(\boldsymbol{x}_i|\boldsymbol{\theta})$ and according to assumption of observation exchangeability [15] the joint prior distribution is given as

$$p(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n, \boldsymbol{\theta}) = \left(\prod_{i=1}^{n} f(\boldsymbol{x}_i|\boldsymbol{\theta}) \right) p(\boldsymbol{\theta}). \tag{3.3}$$

and the posterior as

$$p(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n, \boldsymbol{\theta} | \boldsymbol{z}_1, \ldots, \boldsymbol{z}_n) \propto \left(\prod_{i=1}^{n} f(\boldsymbol{z}_i | \boldsymbol{x}_i) \right) \left(\prod_{i=1}^{n} f(\boldsymbol{x}_i | \boldsymbol{\theta}) \right) p(\boldsymbol{\theta}). \tag{3.4}$$

Our knowledge about the hyperparameters grows by updating based on every new measurement while structure of the model parameters' prior distribution remains unchanged. Hence the Bayesian inference is focused on the hyperparameters $\boldsymbol{\theta}$ and the model parameters $\boldsymbol{x}$ represent nuisance parameters which can be integrated out to get marginal distribution of $\boldsymbol{\theta}$. The marginalized likelihood function is defined as

$$f(\boldsymbol{z}_1, \ldots, \boldsymbol{z}_n | \boldsymbol{\theta}) = \prod_{i=1}^{n} \int f(\boldsymbol{z}_i | \boldsymbol{x}_i) f(\boldsymbol{x}_i | \boldsymbol{\theta}) \mathrm{d}\mathbb{P}(\boldsymbol{x}_i). \tag{3.5}$$

and the corresponding marginalized posterior distribution is simplified into

$$p(\boldsymbol{\theta} | \boldsymbol{z}_1, \ldots, \boldsymbol{z}_n) \propto f(\boldsymbol{z}_1, \ldots, \boldsymbol{z}_n | \boldsymbol{\theta}) p(\boldsymbol{\theta}). \tag{3.6}$$

The integration usually cannot be done analytically thus some integration rule has to be employed to marginalized the likelihood which leads to approximation error and it makes MCMC sampling of the marginalized posterior very computationally demanding. On the other side to sample from the joint distribution is more complicated and requires some advanced MCMC technique [6].

CHAPTER 4

TRANSFORMATION OF RANDOM VARIABLES

The developed method is initially inspired by the Bayesian inference where all the available information are combined in resulting updated distribution of the parameters. As it is focused on the quantification of irreducible uncertainty in the data, the influence of the prior information is suppressed and an non-informative uniform prior PDF is employed. We focus especially on information involved in the experimental data and description of their corresponding joint PDF simultaneously defining the joint distribution of the parameters. The underlying problem of its practical application to real experimental data is an appropriate formulation of the function representing the distribution of the experimental measurements.

This identification procedure allows to deal with a situation where available observations are obtained within a set of experiments, each performed on a different set of specimens (as the experiments are supposed to be destructive). This is a common situation when one type of loading regime (uniaxial tension or compression) does not activate all the material parameters to be identified. Therefore multiple experiments for different loading scenarios are performed to ensure the complete calibration of the material model. Simple multiplication of PDFs constructed for the data from each experiment may lead to underestimating the parameter variance due to underlying assumption of independence among observations from different experiments. Despite the independence of specimens, the observations may be correlated due to their physical meaning described by the material model and hence their dependence on the same material parameters (as e.g. deflection in the uniaxial compression and uniaxial tensile tests depends on Young's modulus and Poisson's ratio).

Therefore the proposed method aims at estimating the intrinsic mutual correlations among the observed quantities, which needs to be done in one of the two following ways. In case of two observations obtained within one type of experiment (e.g. as two points of one measured load-displacement curve), the correlation can be derived directly from the data

(from a set of measured curves we extract a set of paired points and compute the correlation between two obtained columns). In case of two observations obtained from two different experiments, which are performed on different specimens, the correlation cannot be computed directly from the data, since the observations cannot be paired. The correlation is thus estimated from simulated pseudo-data, where two experiments are simulated for the same specimens using some prior distributions of material properties. Of course, the prior distribution can be significantly different from the parameter distribution in real specimens, which may to certain extent affect the estimate of the correlation. Nevertheless, when the data do not allow to estimate the correlation, the pseudo-data provide at least an approximate estimate which includes the information about the relationship among the observations given by physical meaning described by the model.

Once the correlations are estimated, the proposed methodology proceeds to transformation of the data by principal component analysis (PCA) into a set of uncorrelated quantities [31], so called principal components. The principal components are sorted in decreasing order of their variances corresponding to the eigenvalues of the covariance matrix of the data. The first few components account for most of the statistical variability in all of the original data. PCA allows us to reduce the dimensionality of observed data consisting of a large number of correlated variables, while retaining as much as possible of the variation present in the data. Fig. 4.1 shows a simple example of PCA in two dimensions.

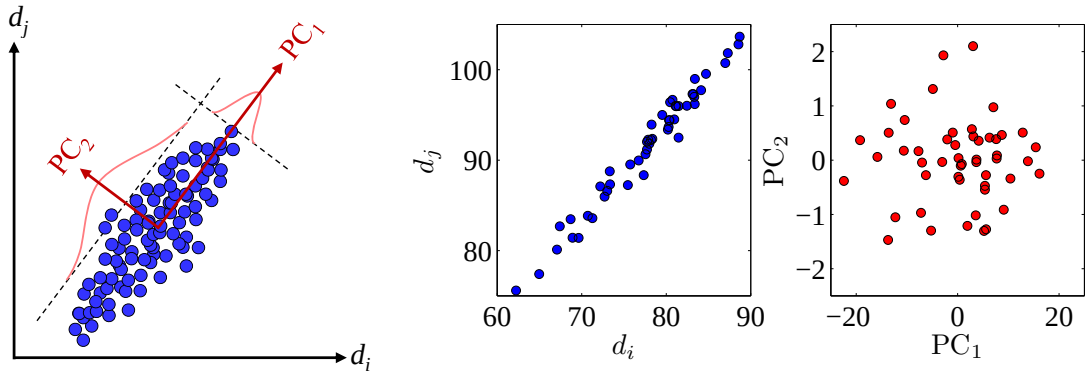


Figure 4.1: An example of principal component analysis.

Considering only a reasonable number of the principal components in the stochastic model updating procedure, it specifically means a reduction of the data dimension to the dimension of the material parameters, which allows to look at the inverse problem as at the nonlinear transformation of random variables. In other words, the problem is reformulated in a way, where we search for a joint distribution of material model parameters, which is given by the joint distribution of principal components obtained from the observations and the nonlinear transformation defined by the material model. For this point of view, the number of considered principal components requires to be equal to the number of identified material parameters. Moreover, principal components are easier to be handled than original response components thanks to their limited number and uncorrelation. And on top of

that, the transformation into principal components also allows eliminating the influence of experimental errors to a certain extent.

Having numerical models of parameters $\boldsymbol{x}$ for all n types of experiments

$$\begin{aligned} \boldsymbol{y}_1 &= g_1(\boldsymbol{x}) \\ &\vdots \qquad , \\ \boldsymbol{y}_n &= g_n(\boldsymbol{x}) \end{aligned} \tag{4.1}$$

the principal components $\boldsymbol{P}$ are the linear combinations of the responses $\boldsymbol{Y}$, i.e.

$$\boldsymbol{P} = h(\boldsymbol{Y}_1, ..., \boldsymbol{Y}_n) = h(g_1(X_1, ..., X_k), ..., g_n(X_1, ..., X_k)). \tag{4.2}$$

The joint distribution of $\boldsymbol{P}$ is considered as a product of marginal univariate PDFs of each P under assumption of the $\boldsymbol{P}$ independence. Finally the searched joint distribution of the parameters has the following formulation based on the multivariate transformation from the random $\boldsymbol{P}$ to the identified parameters as

$$f_{X_1,...,X_k} = f_{PC_1,...,PC_k}(h(g_1(\boldsymbol{X}), ..., g_n(\boldsymbol{X})) \cdot |J_{PC_1,...,PC_k}(X_1, ..., X_k)|, \tag{4.3}$$

where $J_{PC_1,...,PC_k}(X_1, ..., X_k)$ denotes the Jacobian determinant of $\boldsymbol{P}$, it is the determinant of the Jacobian matrix containing all first-order partial derivatives of $\boldsymbol{P}$, i.e.

$$J_{PC_1,...,PC_k}(X_1, ..., X_k) = \det \begin{bmatrix} \frac{\partial PC_1}{\partial x_1} & \frac{\partial PC_1}{\partial x_2} & \dots & \frac{\partial PC_1}{\partial x_k} \\ \frac{\partial PC_2}{\partial x_1} & \frac{\partial PC_2}{\partial x_2} & \dots & \frac{\partial PC_2}{\partial x_k} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial PC_k}{\partial x_1} & \frac{\partial PC_k}{\partial x_2} & \dots & \frac{\partial PC_k}{\partial x_k} \end{bmatrix}. \tag{4.4}$$

Samples of the identified PDF are obtained by the MCMC sampling procedure. In order to accelerate this process, the approximation of the model responses based on PC is employed. The convergence of the approximation error with the increasing number of polynomial terms is optimal in case of orthogonal polynomials of a special type corresponding to the probability distribution of the underlying variables [62]. Since the prior distribution of the parameters is established as uniform, the Legendre polynomials are appropriate to be used in this approach. The polynomial approximation is efficient not only in terms of time requirements, but also for the evaluation of partial derivatives in the Jacobian of the transformation.

CHAPTER 5

POLYNOMIAL CHAOS EXPANSION

In order to accelerate the sampling procedure in the identification process, the evaluations of a numerical model

$$\boldsymbol{y} = g(\boldsymbol{x}), \tag{5.1}$$

can be replaced by evaluations of a model surrogate. In particular, we search for an approximation of the response $\boldsymbol{y}$ by polynomial chaos (PC) expansion [59, 27, 37, 56], which has the following form:

$$\tilde{\boldsymbol{y}}(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha} \in \mathcal{J}} \boldsymbol{\beta}_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{x}), \tag{5.2}$$

where $\boldsymbol{\beta}_{\boldsymbol{\alpha}}$ is a vector of PCE coefficients $\beta_{\boldsymbol{\alpha},i}$ corresponding to a particular component of the system response y_i. $\psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$ are multivariate polynomials and $\boldsymbol{\alpha}$ is a vector of degrees of particular parameters from the index set $\mathcal{J} \subset \mathbb{N}_0$ of non-negative integer sequences with only finitely many non-zero terms, i.e. multi-indices,

$$\mathcal{J} = \{\boldsymbol{\alpha} \in \mathbb{N}^{n_x}, |\boldsymbol{\alpha}| \leq p\}, \tag{5.3}$$

where $|\boldsymbol{\alpha}| = \sum_i^{n_x} \alpha_i$ and p is the maximal degree of polynomials. The expansion (5.3) is usually truncated to the limited number of terms n_β, which is very often related to the number of random variables n_x and to p according to the relation

$$n_\beta = \frac{(p + n_x)!}{p! n_x!}. \tag{5.4}$$

PC can be used to approximate the response with respect to probability distribution of the random variables. There are different base of orthogonal polynomials associated with special types of the probability distribution of the underlying variables [62], e.g. Hermite polynomials are associated with the Gaussian distribution, Legendre polynomials with the uniform distribution and so on.

Polynomial chaos-based surrogate modelling enables to compute statistical moments of an approximated model response analytically from the PC coefficients [61]. In particular, mean can be computed as

$$\mu_{\tilde{r}} = \mathbb{E}[\tilde{r}] = \int \sum_{|\alpha| \leq n_{\mathrm{p}}} \beta_\alpha \psi_\alpha(\boldsymbol{x}) \mathrm{d}\mathbb{P}(\boldsymbol{x}) = \beta_0 \tag{5.5}$$

and standard deviation as

$$\sigma_{\tilde{r}} = \sqrt{\mathbb{E}[(\tilde{r} - \mu_{\tilde{r}})^2]} = \sqrt{\sum_{0<|\alpha| \leq n_{\mathrm{p}}} \mathbb{E}[\psi_\alpha^2(\boldsymbol{x})] \beta_\alpha^2}, \tag{5.6}$$

where

$$\mathbb{E}[\psi_\alpha^2(\boldsymbol{x})] = \int \psi_\alpha^2(\boldsymbol{x}) \mathrm{d}\mathbb{P}(\boldsymbol{x}) = \int \cdots \int_{n_x} \prod_{j=1}^{n_x} (\psi_{\alpha,j}^2(x_j)) \mathrm{d}\mathbb{P}(x_1) \cdots \mathrm{d}\mathbb{P}(x_{n_x}). \tag{5.7}$$

The efficiency of this method thus depends mainly on the computational demands of the PC construction and its accuracy, which are connected with a method chosen for the construction of the surrogate model [46, 42, 2].

There are several methods for construction of PC-based surrogates: linear regression [9, 11, 13], stochastic collocation methods [4, 60] and the stochastic Galerkin method [24, 5, 38, 16]. The principal differences among these methods are following. The linear regression is a stochastic method based on a set of model simulations performed for a stochastic design of experiments, usually obtained by Latin Hypercube Sampling. The PC coefficients are then obtained by regression of the model outputs at the design points, which leads to a solution of a system of equations. On the other side the stochastic collocation method is a deterministic method, which uses a set of model simulations on a sparse grid constructed for a chosen level of accuracy. The computation of the PC coefficients is based on an explicit formula. The stochastic Galerkin method is also deterministic, but leads to a solution of a large system of equations and needs an intrusive modification of the numerical model itself [18, 47].

5.1 Linear regression

A very general method of computing PC coefficients in Eq. (5.2) is a well-known linear regression [9]. The underlying assumption of linear regression is that the surrogate $\tilde{\boldsymbol{y}}$ is a linear combination of the parameters $\boldsymbol{\beta}$, but does not have to be linear in the independent variables $\boldsymbol{x}$. The application is based on the three following steps:

i preparation of data $\mathbf{X} \in \mathbb{R}^{n_x \times n_{\mathrm{d}}}$ which are obtained as n_{d} samples of parameter vector $\boldsymbol{x}_i$

ii evaluation of the model for samples $\boldsymbol{x}_i$ resulting in response samples $\boldsymbol{y}_i$ organised into

the matrix $\mathbf{Y} \in \mathbb{R}^{n_y \times n_\mathrm{d}}$, where n_y is a number of response components and

iii computation of PC coefficients $\boldsymbol{\beta}_\alpha$ organised into the matrix $\mathbf{B} \in \mathbb{R}^{n_y \times n_\beta}$ using e.g. the ordinary least square method.

Since the most time-consuming part of this method consists in evaluations of the model for samples of random variables, the choice of these samples represents a crucial task with the highest impact on the computational time requirements. The simplest way is to choose the samples by Monte Carlo method, i.e. to draw them randomly from the prescribed probability distribution. However, the accuracy of the resulting surrogate depends on a quality, how the samples cover the defined domain [29]. The same quality can be achieved by a smaller number of samples when drawn according to some stratified procedure called design of experiments (DoE). Latin hypercube sampling (LHS) is a well-known DoE able to respect the prescribed probability distributions. There exist also more enhanced ways of optimising the LHS (see e.g. [30]).

The computation of the PC coefficients $\mathbf{B}$ starts by evaluation of all the polynomial terms ψ_α for all the samples $\boldsymbol{x}_i$ and saving them in the matrix $\mathbf{Z} \in \mathbb{R}^{n_\mathrm{d} \times n_\beta}$. The ordinary least square method then leads to

$$\mathbf{Z}^\mathrm{T}\mathbf{Z}\mathbf{B}^\mathrm{T} = \mathbf{Z}^\mathrm{T}\mathbf{Y}^\mathrm{T}, \tag{5.8}$$

which is n_y linear systems of n_β equations.

CHAPTER 6

SENSITIVITY ANALYSIS

Global sensitivity analysis (SA) is an important tool for investigating the relationship between the model inputs and model outputs. In parameter identification it can be used to determine the most sensitive component of the model response to the identified parameter. In other words, it specifies the most suitable quantity to be measured in order to increase efficiency of the identification. This is a basic information for planning the laboratory experiments.

Several approaches to SA have been developed, see e.g. [52]. Widely used sampling-based approaches aim at an evaluation of Spearman's rank correlation coefficient (SRCC) or Sobol' indices based on simulations performed for the design of experiments. Another approach is to use effectively the mentioned polynomial approximation which allows to evaluate the sensitivity in the form of Sobol' indices analytically from its coefficients [10].

The SRCC is able to determine the relationship between the inputs and outputs of nonlinear monotonic models [28] and is computed according to

$$\rho_{x_i,y_j} = 1 - \frac{6\sum_{a=1}^{n}\left(r(x_{i,a}) - r(y_{j,a})\right)^2}{n(n^2-1)}\,, \tag{6.1}$$

where $x_{i,a}$ is a value of the parameter x_i corresponding to a-th model simulation and $y_{j,a}$ is a corresponding model response, n is a total number of the model simulations. The samples $x_{i,a}$ and $y_{j,a}$ are sorted according to their values which gives them the appropriate ranks $r(x_{i,a})$ a $r(y_{j,a})$ used in the computation of the SRCC.

Sobol' indices allow to describe the relationship between the inputs and outputs also for non-monotonic models. The index is a ratio of the output variance induced by a chosen parameter and the total output variance and can be computed from the PC approximation according to

$$S_{x_i} = \frac{\sum_{\boldsymbol{\alpha}\in\mathcal{I}_i}\beta_\alpha^2\mathbb{E}[\psi_{\boldsymbol{\alpha}}^2(\boldsymbol{x})]}{\sum_{\boldsymbol{\alpha}\in\mathcal{J}\setminus\{\mathbf{0}\}}\beta_{\boldsymbol{\alpha}}^2\mathbb{E}[\psi_{\boldsymbol{\alpha}}^2(\boldsymbol{x})]}, \tag{6.2}$$

where $\mathcal{I}_i$ determines the polynomials involving the terms depending only on x_i and polyno-

mial degrees of other variables are null, i.e.

$$\mathcal{I}_i = \{\boldsymbol{\alpha} \in \mathbb{N}^{n_x} : 0 \leq \sum_{j=1}^{s} \alpha_j \leq p, \alpha_l = 0 \iff l \notin (i), \forall l = 1, \ldots, n_x\}, \tag{6.3}$$

and specifically for Legendre polynomials

$$\mathbb{E}[\psi^2_{\boldsymbol{\alpha}}(\boldsymbol{x})] = \int \psi^2_{\boldsymbol{\alpha}}(\boldsymbol{x}) \mathrm{d}\mathbb{P}(\boldsymbol{x}) = \int \cdots \int_{n_x} \prod_{j=1}^{n_x} (\psi^2_{\alpha,j}(x_j)) \mathrm{d}\mathbb{P}(x_1) \cdots \mathrm{d}\mathbb{P}(x_{n_x}) = \prod_{j=1}^{n_x} \frac{2}{2\alpha_j + 1}, \tag{6.4}$$

where α_j is a polynomial degree of variable x_j in the polynomial $\psi_{\boldsymbol{\alpha}}$.

We introduce a simple new type of Sobol indices, so-called additive sensitivity indices, which consist of the sensitivity indices of the considered variable and a part of the sensitivity indices corresponding to the variable's combination with another variables, these indices are divided by the number of appeared variables to get their particular part. The formula for the additive sensitivity indices is

$$S^*_{x_i} = \frac{\sum_{\boldsymbol{\alpha} \in \mathcal{I}_i} \beta^2_{\boldsymbol{\alpha}} \mathbb{E}[\psi^2_{\boldsymbol{\alpha}}(\boldsymbol{x})] + \sum_{\boldsymbol{\alpha} \in \mathcal{I}^*_i} {}^1\!/_{n^*_i} \beta^2_{\boldsymbol{\alpha}} \mathbb{E}[\psi^2_{\boldsymbol{\alpha}}(\boldsymbol{x})]}{\sum_{\boldsymbol{\alpha} \in \mathcal{J} \setminus \{\mathbf{0}\}} \beta^2_{k,\boldsymbol{\alpha}} \mathbb{E}[\psi^2_{\boldsymbol{\alpha}}(\boldsymbol{x})]}, \tag{6.5}$$

where n^*_i is a number of variables included in the polynomials from the set $\mathcal{I}^*_i$ defining all the polynomials involving x_i except the polynomials from $\mathcal{I}_i$, i.e.

$$\mathcal{I}^*_i = \{\boldsymbol{\alpha} \in \mathbb{N}^{n_x} : 0 \leq \sum_{j=1}^{s} \alpha_j \leq p, \boldsymbol{\alpha}_i \neq 0 \ \wedge \boldsymbol{\alpha}_l \neq 0 \iff l \neq i, \forall l = 1, \ldots, n_x\}. \tag{6.6}$$

The total sum of the additive sensitivity indices is equal to one.

CHAPTER 7

NUMERICAL EXAMPLES

The developed identification method based on transformation of random variables has been applied for calibration of several numerical models. In this statement, three of them are presented.

7.1 Affinity hydration model

Affinity hydration models provide a framework for accommodating all stages of cement hydration. We consider hydrating cement under isothermal temperature 25°C. At this temperature, the rate of hydration can be expressed by the chemical affinity $\tilde{A}_{25}(\alpha)$ under isothermal 25°C

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = \tilde{A}_{25}(\alpha), \tag{7.1}$$

where the chemical affinity has a dimension of time^{-1} and α stands for the degree of hydration.

The affinity for isothermal temperature can be obtained experimentally; isothermal calorimetry measures a heat flow $q(t)$ which gives the hydration heat $Q(t)$ after integration. The approximation is given

$$\frac{Q(t)}{Q_{pot}} \approx \alpha, \tag{7.2}$$

$$\frac{1}{Q_{pot}}\frac{\mathrm{d}Q(t)}{\mathrm{d}t} = \frac{q(t)}{Q_{pot}} \approx \frac{\mathrm{d}\alpha}{\mathrm{d}t} = \tilde{A}_{25}(\alpha), \tag{7.3}$$

where Q_{pot} is expressed in J/g of cement paste. Hence the normalized heat flow $\frac{q(t)}{Q_{pot}}$ under isothermal 25°C equals to chemical affinity $\tilde{A}_{25}(\alpha)$.

Cervera et al. [12] proposed an analytical form of the normalized affinity which was

refined in [21]. Here we use a slightly modified formulation [58]:

$$\tilde{A}_{25}(\alpha) = B_1 \left(\frac{B_2}{\alpha_\infty} + \alpha \right) (\alpha_\infty - \alpha) \exp\left(-\eta \frac{\alpha}{\alpha_\infty} \right), \tag{7.4}$$

where B_1, B_2 are coefficients related to chemical composition, when

$$B_2 = \frac{(-0.0767 \cdot C_4AF + 0.0184) \cdot B_f}{B_1 \cdot 350}, \tag{7.5}$$

where Blaine fineness $B_f = 392.5\mathrm{m}_2/\mathrm{kg}$ and mass percentage of C_4AF is 10%. α_∞ is the ultimate hydration degree and η represents microdiffusion of free water through formed hydrates.

When hydration proceeds under varying temperature, maturity principle expressed via Arrhenius equation scales the affinity to arbitrary temperature T

$$\tilde{A}_T = \tilde{A}_{25} \exp\left[\frac{E_a}{R} \left(\frac{1}{273.15 + 25} - \frac{1}{T} \right) \right], \tag{7.6}$$

where R is the universal gas constant (8.314 $\mathrm{Jmol}^{-1}\mathrm{K}^{-1}$) and E_a [Jmol^{-1}] is the activation energy. For example, simulating isothermal hydration at 35°C means scaling $\tilde{A}_{25}$ with a factor of 1.651 at a given time. This means that hydrating concrete for 10 hours at 35°C releases the same amount of heat as concrete hydrating for 16.51 hours under 25°C. Note that setting $E_a = 0$ ignores the effect of temperature and proceeds the hydration under 25°C. The evolution of α is obtained through numerical integration since there is no analytical exact solution.

The goal of this example is to identify parameters B_1, α_∞ and η from 50 pseudo-experimental α curves. Uninformative uniform prior distribution is defined by its bounds given in Tab. 7.1.

Parameter	Minimum	Maximum
B_1 [h^{-1}]	0.1	1.0
η [−]	2.0	12.0
α_∞ [−]	0.7	1.0

Table 7.1: Bounds for affinity model parameters.

At first, the given data are transformed into the principal components and the first three of them are considered in the identification process. PC approximation in the form of fourth order Legendre polynomials is employed. Fig. 7.1 depicts results of sensitivity analysis based on additive sensitivity indices for the principal components computed from the PC coefficients.

The marginal distribution of each principal component is formulated as normal kernel estimation from the transformed data. Their joint distribution is transform by the appropriate Jacobian into the joint distribution of the parameters. Fig. 7.2 shows the resulting para-

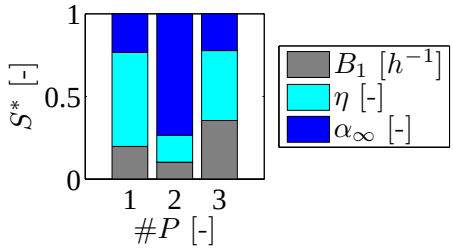


Figure 7.1: Additive sensitivity indices expressing influence of each model parameter to the principal components.

meters' distribution obtained from 100,000 MCMC samples as marginal univariate, resp. bivariate PDFs.

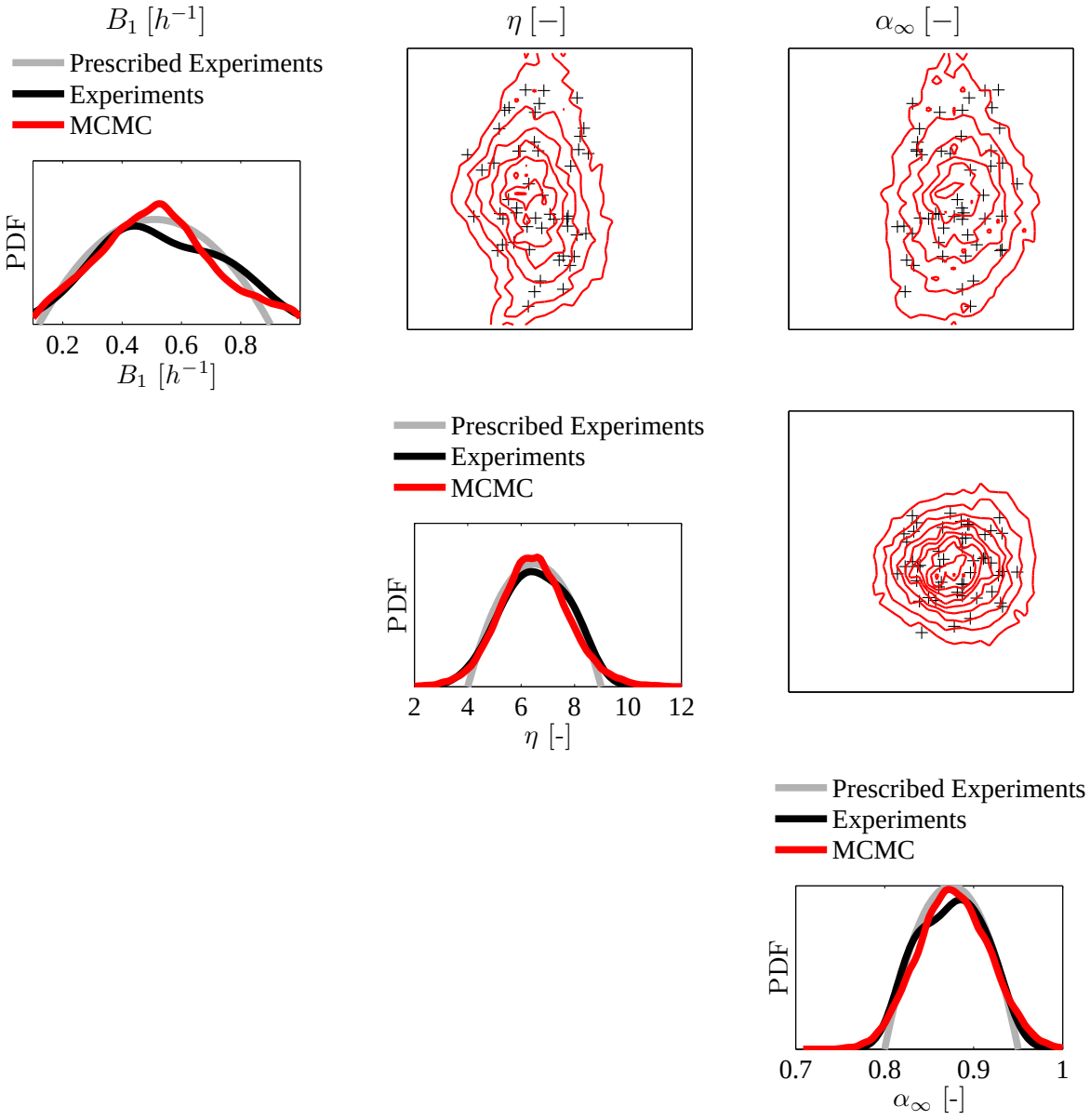


Figure 7.2: Identified univariate and bivariate distribution of particular parameters.

To validate the identification, the model response corresponding to the identified parameters' PDF is compared to the pseudo-experimental data in Fig. 7.3. There we get a very

good fit and can conclude that the identification process is successful.

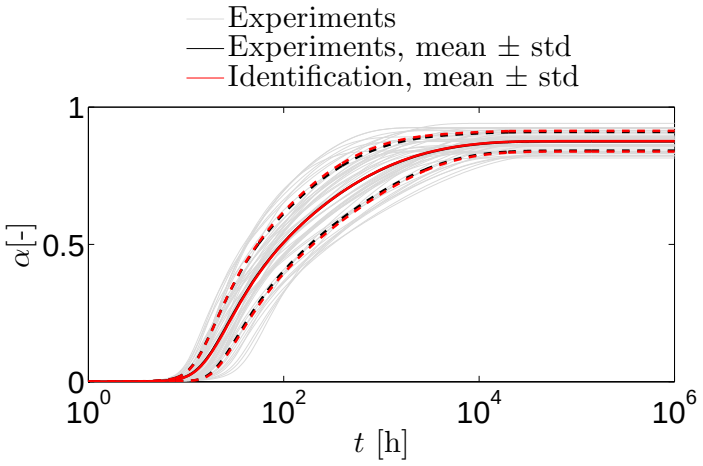


Figure 7.3: Comparison of pseudo-experimental data and model response corresponding to the identified parameters' PDF.

7.2 Parameter identification from cyclic loading test

The second numerical example is a part of the ESA project Reliability Analysis and Life Prediction with Probabilistic Methods. For this reason, the detailed information and results are confidential therefore all the numerical data are scaled. We obtained a pseudo-experimental set of 50 curves from the cyclic loading test of a heterogeneous viscoplastic material, see Fig. 7.4. The response of corresponding numerical model is influenced by six uncertain parameters and the model itself is considered as a black box. The given data set is produced for inputs where two of the parameters are strongly correlated. Task is to identify the relevant parameters within the given loading test and their probability density functions (PDF) corresponding to the measured experimental curves.

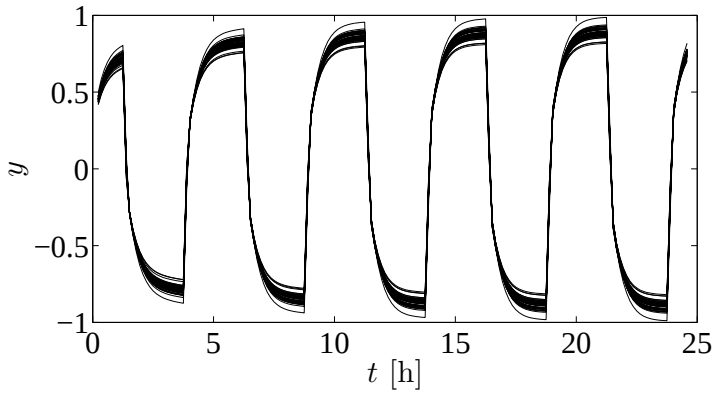


Figure 7.4: Given pseudo-experimental curves.

The obtained data are transformed into the principal components and the first six of them are considered in the identification process. PC approximation in the form of sixth order

Legendre polynomials is employed. The marginal distribution of each principal component is formulated as normal distribution with mean value and standard deviation estimated from the transformed data. The defined joint distribution is transform by the appropriate Jacobian into the joint distribution of the parameters.

The parameters' marginal univariate and bivariate PDFs obtained by normal kernel estimation from the $500,000$ MCMC samples are shown in Fig. 7.5 and the correlation matrix corresponding to the whole joint distribution is given in Eq. 7.7. Results confirm that the proposed method is able to identified introduced correlation between parameters x_1 and x_2 in the experimental samples.

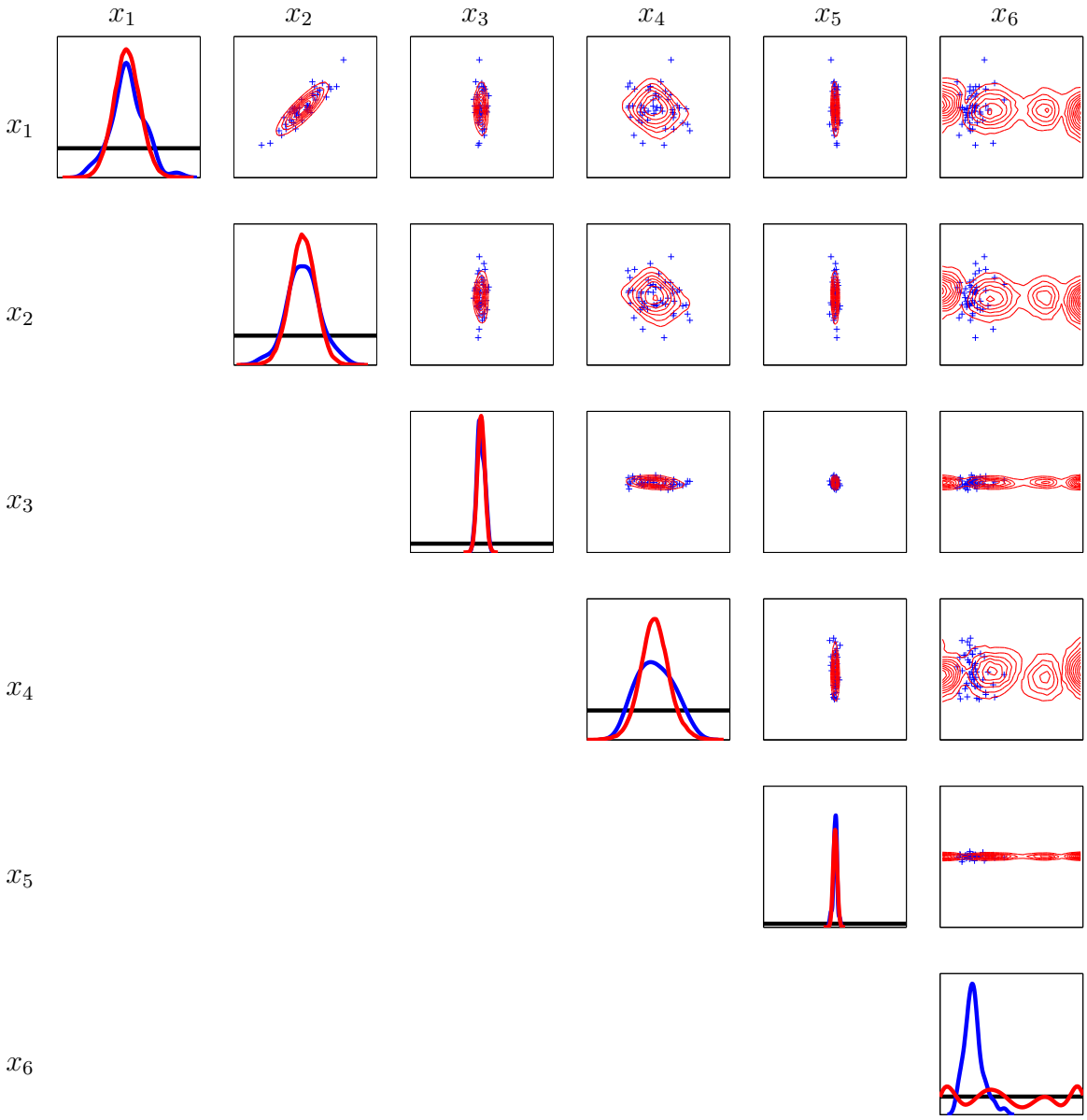


Figure 7.5: Identified 1D and 2D marginal pdfs of model parameters (red) and experimental samples (blue).

$$\mathbf{R} = \begin{pmatrix} 1.000 & 0.868 & -0.034 & -0.198 & -0.149 & -0.225 \\ 0.868 & 1.000 & 0.016 & -0.248 & -0.075 & -0.238 \\ -0.034 & 0.016 & 1.000 & -0.235 & -0.047 & 0.028 \\ -0.198 & -0.248 & -0.235 & 1.000 & -0.022 & 0.031 \\ -0.149 & -0.075 & -0.047 & -0.022 & 1.000 & 0.045 \\ -0.225 & -0.238 & 0.028 & 0.031 & 0.045 & 1.000 \end{pmatrix} \tag{7.7}$$

In Fig. 7.6 the model output corresponding to the identified parameters' distributions is compared to the experimental data.

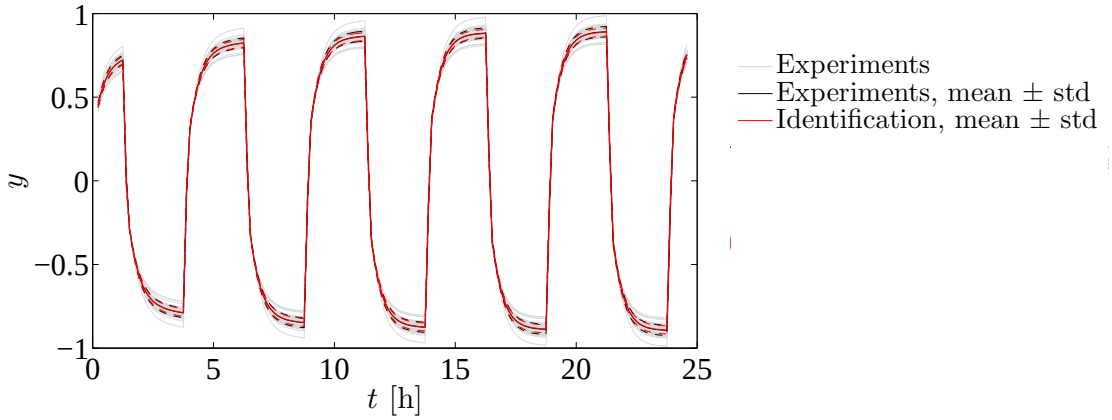


Figure 7.6: Comparison of experimental data and model response corresponding to the identified parameters.

The parameter ν is not identified. This can be caused by small sensitivity of the output to this parameter, this assumption is confirmed by results of sensitivity analysis given in Fig. 7.7. The sensitivity determine the relevant and irrelevant parameters within given loading test. Now we express the sensitivity of stress to particular parameters with help of SRCC. The sensitivity is calculated from $50,000$ samples of prior parameters' PDFs. We can conclude that ν is the irrelevant parameter.

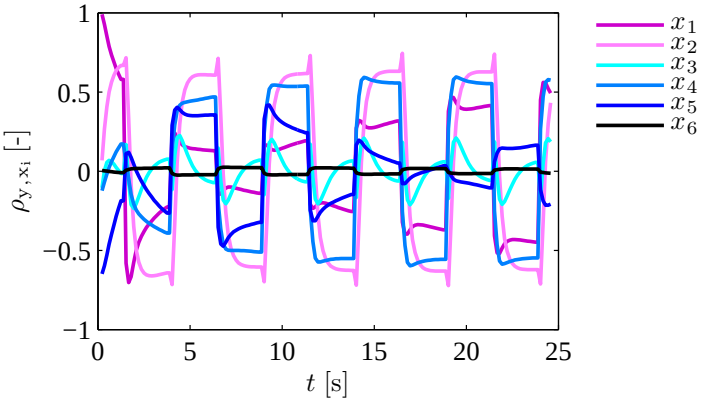


Figure 7.7: Sensitivity analysis of dependence between the parameters and stress.

7.3 Calibration of damage model

This example concentrates on stochastic parameter identification of heterogeneous materials from different types of destructive experiments.

The proposed identification method is applied at identification of material parameters of a damage model derived from the Landgraf Morrow equation. The relation between the strain range $\Delta\varepsilon$ and the number of cycles to a failure of the specimen N_f is given as

$$N_f = \left(\frac{\Delta\varepsilon}{S}\right)^{-s}. \tag{7.8}$$

The material parameters to be identified are the fatigue ductility coefficient S [-] and fatigue ductility exponent s [-]. The expert knowledge about these parameters is formulated as an non-informative prior uniform distribution on the intervals from 0.1 to 1.2 for S and from 1.0 to 2.8 for s.

In order to identify the damage parameters, two types of destructive experiments are considered and only pseudo-experimental data are used in this study. The first experiment is a tensile test with 50 repetitions, where the measured quantity is the strain at rupture and directly corresponds to the identified parameter S. In the second experiment with 30 realizations, the number of cycles to a failure of the specimen N_f is measured under cyclic loading with the strain range $\Delta\varepsilon = 0.03$. The histograms of the pseudo-experimental data and the corresponding marginal distributions are depicted in Fig. 7.8.

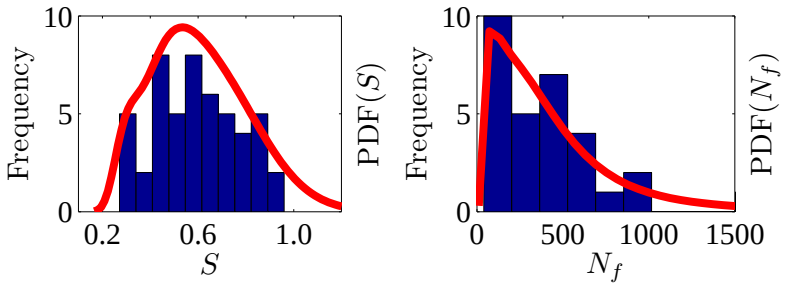


Figure 7.8: Distributions of pseudo-experimental observations.

The application of the developed method having data from different sets of specimens requires involving information about mutual correlations based on the prior parameters' PDF. Knowledge of these mutual correlations and marginal distribution estimates of the particular measurements based on a normal kernel function enables us to produce new synthetic experimental samples. The joint distribution of $\boldsymbol{P}$ is constructed on the basis of 10.000 synthetic samples and subsequently transformed by the appropriate Jacobian to the joint distribution of the damage parameters. Fig. 7.9 shows identified joint distribution and marginal PDFs of the particular parameters.

The identification of the fatigue ductility coefficient S is essentially perfect, whereas variance of the fatigue ductility exponent s is not identified well. The obtained difference

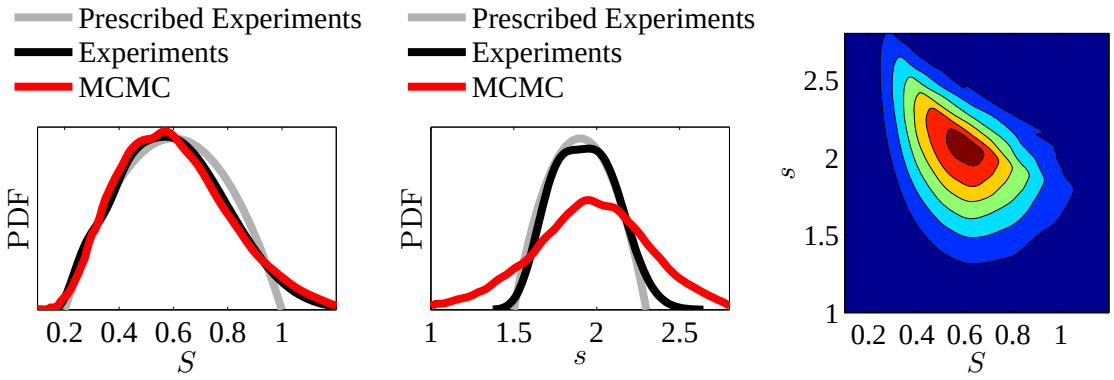


Figure 7.9: Identified parameters' distribution - marginal PDFs and isolines of joint PDF.

in the variance of s is probably caused by omission of the $\boldsymbol{PC}$ dependency. The important aspect for assessing the success of the identification method is comparison of the distribution of the given data and the distribution of the model responses corresponding to the identified parameters' PDF. In this context the identification is successful, see Fig. 7.10.

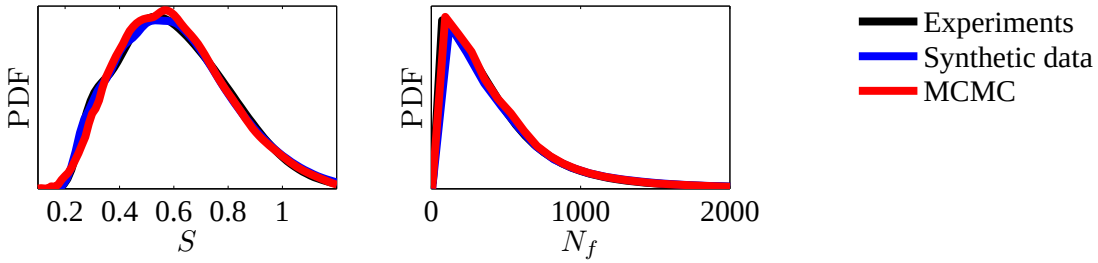


Figure 7.10: Comparison of experimental observations and model responses corresponding to the identified parameters' distribution.

CHAPTER 8

CONCLUSION

The submitted statement represents a thematic overview of the doctoral thesis dealing with identification of aleatory uncertainty in parameters of heterogeneous materials. The research focuses on methodology which enables to find a probability distribution of the model parameters providing a distribution of the model response corresponding to the distribution of the observed data.

During previous part of the doctoral studies, a new identification procedure was developed. The proposed methodology recasts the inverse problem in probabilistic framework similar to Bayesian inference. The principal idea is to formulate the inverse problem as a nonlinear transformation of joint distribution of observed quantities into the corresponding joint distribution of material model parameters. The crucial step of the method concerns the proper formulation of the joint distribution of the observed data. Computationally, the method is based on MCMC sampling of the prescribed joint distribution. It is computationally reasonable, especially in combination with the PC-based surrogate of the material model. The method allows to combine data from different types and numbers of experiments with the inclusion of dependencies among the experiments. In contrast to methods commonly found in the literature, the principal advantage of the method consists in no preliminary assumptions about a specific type of parameters' PDF. On the other side, a significant drawback of the identification procedure is its inability to distinguish between aleatoric and epistemic uncertainties, the method identifies the both types of uncertainties together. A part of this statement is validation of the developed methodology on parameter identification of three material models.

The presented stochastic inversion arises from formulation of the data distribution. Therefore, the procedure is limited to cases with large data sets, which allow to determine the corresponding statistical model with a negligible uncertainty. In case of a very low number of experiment repetitions, the underlaying epistemic uncertainty needs to be considered. The aim of the current research is to separate the aleatory and epistemic uncertainty

by methodology that allows a minimisation of the latter along with the quantification of the former. We plan to focus on Bayesian hierarchical modelling of uncertainties, where statistical moments are modelled as random variables and can be updated for any new observation. So as to avoid the necessity to assume a particular family of statistical models, PC will be employed again to allow for representation of non-Gaussian variables. Analogically, the PC expansion will be employed to describe the PDF of material parameters and corresponding PC coefficients will be considered as uncertain. The distribution of PC coefficients will thus quantify the epistemic uncertainty in the resulted estimation of material parameters' PDF.

The objective of the doctoral thesis is to review, compare and extend the available methods for identification of inherent variability (aleatory uncertainties) with application in calibrating heterogeneous material models.

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