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# Adaptive method for indirect identification of the statistical properties of random fields in a Bayesian framework

Guillaume Perrin · Christian Soize

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Abstract This work considers the challenging problem of identifying the statistical properties of random fields from indirect observations. To this end, a Bayesian approach is introduced, whose key step is the nonparametric approximation of the likelihood function from limited information. When the likelihood function is based on the evaluation of an expensive computer code, this work also proposes a method to sele
t iteratively new design points to reduce the uncertainties on the results that are due to the approximation of the likelihood. Two applications are finally presented to illustrate the efficiency of the proposed procedure: a first one based on analytic data, and a second one dealing with the identification of the random elasticity field of an heterogeneous mi
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ture.

Keywords Bayesian framework  $\cdot$  uncertainty quantification  $\cdot$  statistical inferen
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ess · kernel density estimation

## 1 Introdu
tion

Random field analysis has become a major tool in many scientific fields, such as uncertainty quantification, material science, biology, medicine, signal processing, quantitative finance, etc. However, in most of these applications, the knowledge of these random fields, which we write  $X$ , is limited. Numerical methods are therefore needed to identify the probability distribution of  $X$ from the available information.

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When the information is constituted of direct measurements of the field to model, several te
hniques have been proposed to perform su
h an identi fication. For instance, the AutoRegressive-Moving-Average (ARMA) models [\[Whittle,](#page-25-0) 1951, Whittle, 1983, Box and [Jenkins,](#page-23-0) 1970], allow the description of Gaussian stationary random fields as a parameterized integral of a Gaussian white noise. When onsidering a priori non-Gaussian and nonstationary random fields, the identification is generally based on a two-step procedure. The first step is the approximation of the random field by its projection on a redu
ed number of deterministi fun
tions [\[Ghanem](#page-23-1) and Spanos, 2003, Le [Maître](#page-24-0) and Knio, 2010, using for instance the proper orthogonal decomposition  $[Atwell and King, 2001],$  $[Atwell and King, 2001],$  the proper generalized decomposition  $[Now, 2010],$ or the Karhunen-Loève expansion [\[Williams,](#page-25-2) 2011, Perrin et al., 2014, Perrin et al., 2013]. The second step is the identification of general stochastic representations of the projection coefficients in high stochastic dimension [\[Soize,](#page-25-3) 2010, [Soize,](#page-25-4) 2011, [Perrin](#page-24-4) et al., 2012, Nouy and [Soize,](#page-24-5) 2014, Soize and [Ghanem,](#page-25-5) 2016, Perrin et al., 2018.

The main specificity of this work comes from the fact that only indirect observations are available for the identification, in the sense that the experimental data is made of the transformations of a limited number of independent realizations of  $X$  through a black-box time-consuming nonlinear mapping, denoted by  $g$ . To make this identification tractable, we assume that the random field to identify belongs to a known parametric class. Thus, identifying the distribution of  $\boldsymbol{X}$  amounts to identifying the values of these parameters, which are gathered in the vector  $z$ . A Bayesian framework is then considered [\[Marzouk](#page-24-6) and Najm, 2009[, Stuart,](#page-25-7) 2010, [Arnst](#page-23-3) et al., 2010, [Matthies](#page-24-7) et al., 2016, [Emery](#page-23-4) et al., 2016. parameter  $z$  is supposed to be random, and we search its posterior distribution given the available data.

Markov Chain Monte Carlo (MCMC) [\[Rubinstein](#page-25-8) and Kroese, 2008, Tian et al., 2016] is generally onsidered as a powerful tool to explore the posterior distribution for these parameters. However it an be omputationally prohibitive when ea
h posterior evaluation requires evaluations of a omputationally expensive ode, as it the ase here. To ir
umvent this problem, a standard approa
h is to repla
e the ode by a surrogate model, and to dire
tly sample from the approximated posterior distribution associated with the modified likelihood using classical MCMC procedures. The surrogate model can be based on polynomial rep-resentations [\[Marzouk](#page-24-6) and Najm, 2009, [Marzouk](#page-24-8) and Xiu, 2009, Wan and [Zabaras,](#page-25-10) 2011, Li and [Marzouk,](#page-24-9) 2014, Tsilifis et al., 2017, Gaussian process regression [Kennedy and O['Hagan,](#page-24-10) 2001, [Santner](#page-25-12) et al., 2003,[Higdon](#page-23-5) et al., 2008,Bilionis and [Zabaras,](#page-23-6) 2015, [Sinsbe
k](#page-25-13) and Nowak, 2017, [Damblin](#page-23-7) et al., 2013, or runs of the code at different resolution levels [\[Higdon](#page-23-8) et al., 2003, Chen and Schwab, 2015]. Alternatively, the surrogate model can be used to adapt the proposal distribution. In that ase, the number of expensive posterior evaluations per MCMC step an be strongly redu
ed, while sampling asymptoti
ally from the exa
t posterior distribution (see [\[Rasmussen,](#page-25-14) 2003, [Fielding](#page-23-10) et al., 2011, [Conrad](#page-23-12) et al., 2016, Conrad et al., 2018 for further details about this approa
h).

This work can be seen as an extension of these methods to the case of stochastic codes. Indeed, for a given value of z, as  $X(z)$  is random,  $g(X(z))$ 

is also a random quantity. But if the distribution of  $X(z)$  is known once z is fixed, the distribution of  $g(X(z))$  is unknown, and its identification is omputationally demanding. Therefore, instead of onstru
ting a surrogate model of the code, we focus on the approximation of the probability density function (PDF) of  $g(X(z))$ .

To run a MCMC pro
edure based on the asso
iated approximated likelihood in a reasonable computational time, this approximation of the PDF of  $g(X(z))$  in any z has to be constructed from a fixed number of already computed code evaluations. To this end, we first propose to directly work on the joint PDF of  $(q(X(z)), z)$ . Then, we focus on the Gaussian kernel density esti-mation (G-KDE) [Wand and [Jones,](#page-25-15) 1995, Scott and Sain, 2004, Perrin et al., 2018] for the PDF approximation. Indeed, this method is particularly interesting for its ability to model non-Gaussian distributions with omplex dependen
e structures, but also because it allows an explicit derivation of the PDF of  $g(X(z))|z$  once the joint PDF is known. To construct relevant PDF approximations of this potentially high-dimensional random ve
tor from a reduced number of code evaluations, we finally introduce two adaptations of the lassi
al G-KDE formalism. First, an optimal partitioning of the omponents of  $g(X(z))$  is introduced, which consists in decomposing the random vector to model in well-chosen groups of components that can reasonably be onsidered as independent. Se
ondly, a sequential strategy is proposed to hoose the evaluations points on whi
h the G-KDE relies. Starting from a space-filling design, the objective is to sequentially add new code evaluations in the regions where the posterior distribution of the parameters is high. We refer to [McKay et al., 1979, Fang and Lin, 2003, Fang et al., 2006, Draguljić et al.,  $2012$ [, Joseph](#page-24-12) et al.,  $2015$  for the construction of the initial space-filling designs when the input spaces is an hyperrectangle, and to [\[Stinstra](#page-25-17) et al., 2003, [Stinstra](#page-25-18) et al., 2010, Auffray et al., 2012, Draguljić et al., 2012, [Lekivetz](#page-24-13) and Jones, 2015, Mak and [Joseph,](#page-24-14) 2016, Perrin and [Cannamela,](#page-24-15) 2017 for the general case.

The outline of this work is as follows. Section [2](#page-3-0) presents the theoretical framework of the proposed method. Section [3](#page-10-0) first illustrates the efficiency of the method on an analyti
al example, and then shows its potential for the identification of the mechanical properties of an unknown heterogeneous

## <span id="page-3-0"></span>2 Indirect identification of the statistical properties of random fields

The objective of this section is to describe the adaptive procedure we propose for the identification of the statistical properties of random fields when the available information is a set of indire
t observations.

2.1 Definitions and notations

Let  $(\Omega, \mathcal{A}, \mathbb{P})$  be a probability space. For  $d_x, d_y, d_z \geq 1$ ,

- $\mathcal{P}(\mathbb{X}, \mathbb{R}^{d_x})$  denotes the space of all the second-order random fields defined on  $(\varOmega, \mathcal{A}, \mathbb{P})$ , with values in  $\mathbb{R}^{d_x}$ , indexed by a compact and connected space X;
- $-L^2(\mathbb{X}, \mathbb{R}^{d_x})$  is the space of all the square-integrable functions defined on X with values in  $\mathbb{R}^{d_x}$ ;
- $g$  is a nonlinear measurable mapping whose computational cost can be high:

$$
g: \begin{cases} L^2(\mathbb{X}, \mathbb{R}^{d_x}) \rightarrow \mathbb{R}^{d_y} \\ h \rightarrow g(h) \end{cases} ; \qquad (1)
$$

- $\,\, \mathcal{X}(\mathbb{R}^{d_z},\mathbb{R}^{d_x})$  refers to a particular class of random fields in  $\mathcal{P}(\mathbb{X},\mathbb{R}^{d_x}),$  whose statistical properties are parameterized by a deterministic vector  $\boldsymbol{z} \in \mathbb{R}^{d_z}$ . For instance,  $\mathcal{X}(\mathbb{R}^{d_z}, \mathbb{R}^{d_x})$  can correspond to the set of Gaussian random fields, whose mean and covariance functions are parameterized by the same  $d_z$  coefficients.
- For all  $\boldsymbol{z}$  in  $\mathbb{R}^{d_z}$ ,  $\boldsymbol{X}(\boldsymbol{z})$  is an element of  $\mathcal{X}(\mathbb{R}^{d_z}, \mathbb{R}^{d_x})$ .

Let  $X^*$  be a particular element of  $\mathcal{P}(\mathbb{X}, \mathbb{R}^{d_x})$ , which can belong or not to  $\mathcal{X}(\mathbb{R}^{d_z},\mathbb{R}^{d_x})$ , and  $\boldsymbol{Y}^{\star}$  be its transformation by  $\boldsymbol{g}$ . By construction,  $\boldsymbol{Y}^{\star}$  is a  $d_y$ -dimensional random vector. For each realization of  $\boldsymbol{X}^{\star}$ , which we denote by  $\bm{X}^{\star}(\theta)$  with  $\theta \in \Omega$ ,  $\bm{Y}^{\star}(\theta) := \bm{g}(\bm{X}^{\star}(\theta))$  defines a particular realization of  $Y^*$ .

Given N independent realizations of  $Y^*$ , gathered in the set

$$
\mathcal{S}(N) := \{ \boldsymbol{Y}^{\star}(\theta_n) \}_{1 \le n \le N}, \ \ \theta_n \in \Omega,
$$

the purpose of this work is to propose a Bayesian formalism for the identification of  $z^*$ , such that the probability distribution of  $X(z^*)$  is the closest to the one of  $X^*$ .

### Remarks

- $-$  As mentioned in Introduction, it is important to notice that for each  $z \in$  $\mathbb{R}^{d_z},\,\boldsymbol{g}(\boldsymbol{X}(\boldsymbol{z}))$  is random. This strongly limits the possibility of replacing mapping  $z \mapsto g(X(z))$  by a surrogate model, as it is classically done when solving inverse problems that invoke omputationally expensive models.
- − In the following, for the sake of simplicity, we assume that  $\bm{X}^{\star} \in \mathcal{X}(\mathbb{R}^{d_z}, \mathbb{R}^{d_x})$ . If it was not the case, it could be necessary to introduce an error term to model the difference between  $X^*$  and  $X(z)$  [Kennedy and O['Hagan,](#page-24-10) 2001].

#### 2.2 Bayesian formulation of the problem

In this work,  $z^*$  is modeled by the random vector  $Z$ , to take into account the fact that its value is unknown. Let  $f_Z$  be the probability density function (PDF) of  $Z$ , which is supposed to be known as a prior model. Hence, identifying  $z^*$  amounts to searching the posterior PDF of  $\mathbf{Z} \mid \mathcal{S}(N)$ , which we denote by  $f_{\mathbf{Z}|S(N)}$ . Using the Bayes theorem, it comes:

$$
f_{\mathbf{Z}|S(N)}(z) = \frac{\mathcal{L}_{\mathcal{S}(N)}(z) f_{\mathbf{Z}}(z)}{\mathbb{E}\left[\mathcal{L}_{\mathcal{S}(N)}(\mathbf{Z})\right]}, \ z \in \mathbb{R}^{d_z}.
$$
 (2)

There,  $\mathbb{E}[\cdot]$  is the mathematical expectation and  $\mathcal{L}_{\mathcal{S}(N)}$  is the likelihood function. The elements of  $\mathcal{S}(N)$  being statistically independent, it follows:

$$
\mathcal{L}_{\mathcal{S}(N)}(z) = \prod_{n=1}^{N} f_{\mathbf{Y}(z)}(\mathbf{Y}^{\star}(\theta_n)), \ z \in \mathbb{R}^{d_z},
$$
\n(3)

in which  $f_{\boldsymbol{Y}(\boldsymbol{z})}$  is the PDF of  $\boldsymbol{Y}(\boldsymbol{z}) := \boldsymbol{g}(\boldsymbol{X}(\boldsymbol{z}))$  for given  $\boldsymbol{z}$  in  $\mathbb{R}^{d_z}$ , and is unknown. To approximate  $f_{\boldsymbol{Y}(\boldsymbol{z})},$  a first possibility is to generate  $M$  independent realizations of  $Y(z)$ . Thus, based on this set, the value  $f_{Y(z)}(y)$  of  $f_{Y(z)}$  in any point  $\bm{y}$  in  $\mathbb{R}^{d_y}$  can be approximated using any parametric or nonparametric statistical learning technique. However, this means that function  $g$  has to be evaluated  $M\times Q$  times to evaluate function  $\mathcal{L}_{\mathcal{S}(N)}$  in  $Q$  points for  $\boldsymbol{z}.$  This qui
kly be
omes burdensome when the omputational ost for ea
h evaluation of  $g$  is relatively high (between several minutes to several hours CPU for the considered applications). One possible approach to circumvent this problem is to directly approximate the joint PDF of the  $(d_u + d_z)$ -dimensional random vector  $(Y(Z), Z)$  [Soize and [Ghanem,](#page-25-19) 2017]. Indeed, M independent realizations of  $(Y(Z), Z)$  can be obtained from the following two-step procedure:

- we first draw at random  $M$  independent realizations of  $\boldsymbol{Z}$  according to the distribution  $f_Z$ , which we denote by  $\mathbf{Z}(\omega_1), \ldots, \mathbf{Z}(\omega_M)$ , where  $\omega_1, \ldots, \omega_M$ are in  $\Omega$ :
- for each value of  $\boldsymbol{z}$  in  $\{\boldsymbol{Z}(\omega_1),\ldots,\boldsymbol{Z}(\omega_M)\},$  we draw, at random and independently the ones from the others, a particular realization of  $X(z)$ , and we deduce a realization of  $Y(z)$  by evaluating g in this realization of  $X(z)$ .

For the sake of simplicity, we denote these realizations by  $\mathbf{Y}(\omega_m)$ ,  $1 \leq m \leq$ M. Based on these realizations, the kernel estimator of  $f_{Y,Z}$  is:

$$
\widehat{f}_{\boldsymbol{Y},\boldsymbol{Z}}(\boldsymbol{y},\boldsymbol{z};\boldsymbol{H}) := \frac{\det(\boldsymbol{H})^{-1/2}}{M} \sum_{m=1}^M K\left(\boldsymbol{H}^{-1/2}\left((\boldsymbol{y},\boldsymbol{z}) - (\boldsymbol{Y}(\omega_m),\boldsymbol{Z}(\omega_m))\right)\right).
$$

Here,  $det(\cdot)$  is the determinant operator, K is any positive function whose integral over  $\mathbb{R}^{d_y+d_z}$  is one, and  $\tilde{H}$  is a  $((d_y+d_z) \times (d_y+d_z))$ -dimensional positive-definite symmetric matrix, which is generally referred as the "bandwidth matrix". In the following, we focus on the case where  $K$  is the Gaussian multidimensional density, and where  $H$  is proportional to the empirical estimation of the covariance matrix of  $(Y(Z), Z)$ , denoted by  $\tilde{C}$ :

$$
H = h^2 \hat{C}, \quad h \in \mathbb{R}.\tag{5}
$$

 $\ddot{\phantom{1}}$ 

The main interest of this hypothesis comes from the fact that it strongly reduces the number of parameters that need to be identified for the construction of  $H$ , while generally leading to very interesting results for the modeling of multivariate PDFs (see [\[Perrin](#page-25-6) et al., 2018] for more details). Other parsimonious parameterizations could be proposed for  $H$ , such as diagonal representations, but for sufficiently high values of  $M$ , the influence of this choice on the identification results is expected to be small.

Hence, the PDF of  $(Y(Z), Z)$  is approximated by a mixture of M Gaussian PDFs, for which the means are the available realizations of  $(Y(Z), Z)$  and the ovarian
e matri
es are all parameterized by a unique s
alar h:

$$
\widehat{f}_{\mathbf{Y},\mathbf{Z}}(\mathbf{y},\mathbf{z};h) = \frac{1}{M} \sum_{m=1}^{M} \phi\left((\mathbf{y},\mathbf{z});(\mathbf{Y}(\omega_m),\mathbf{Z}(\omega_m)),h^2\widehat{\mathbf{C}}\right).
$$
 (6)

There, for any  $\mathbb{R}^d$ -dimensional vector  $\boldsymbol{\mu}$  and for any  $(\mathbb{R}^d \times \mathbb{R}^d)$ -dimensional symmetric positive-definite matrix  $C,$   $\phi(\cdot;\bm{\mu},\bm{C})$  is the PDF of any  $\mathbb{R}^d$ -dimensional Gaussian random vector with mean  $\mu$  and covariance matrix  $C$ :

$$
\phi(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{C}) := \frac{\exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{C}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right)}{(2\pi)^{d/2}\sqrt{\det(\boldsymbol{C})}}, \quad \mathbf{x} \in \mathbb{R}^d.
$$
 (7)

In addition, the block decomposition of  $\hat{C}$  is written as:

$$
\hat{C} = \begin{bmatrix} \hat{C}_{YY} & \hat{C}_{YZ} \\ \hat{C}_{YZ}^T & \hat{C}_{ZZ} \end{bmatrix} .
$$
\n(8)

For all  $(\bm{y}, \bm{z}) \in \mathbb{R}^{d_y} \times \mathbb{R}^{d_z}$ , the kernel approximation of  $f_{\bm{Y}(\bm{z})}(\bm{y})$ , which we denote by  $f_{\boldsymbol{Y}(\boldsymbol{z})}(\boldsymbol{y};h)$ , can therefore be written as follows (see Appendix for more details about this expression):

<span id="page-6-0"></span>
$$
\hat{f}_{\mathbf{Y}(z)}(\mathbf{y};h) = \frac{\hat{f}_{\mathbf{Y},\mathbf{Z}}(\mathbf{y},z;h)}{\int_{\mathbb{R}^{d_{y}}} \hat{f}_{\mathbf{Y},\mathbf{Z}}(\mathbf{v},z;h) d\mathbf{v}} = \sum_{m=1}^{M} \frac{\gamma_{m}(z;h)}{\sum_{m'=1}^{M} \gamma_{m'}(z;h)} \phi(\mathbf{y};\boldsymbol{\mu}_{m}(z),\boldsymbol{C}_{m}(h)),
$$
\n(9)

$$
\gamma_m(z;h) := \exp\left(-\frac{1}{2h^2}\left(\boldsymbol{z} - \boldsymbol{Z}(\omega_m)\right)^T \widehat{\boldsymbol{C}}_{\boldsymbol{Z}\boldsymbol{Z}}^{-1}\left(\boldsymbol{z} - \boldsymbol{Z}(\omega_m)\right)\right),\qquad(10)
$$

$$
\mu_m(z) := \mathbf{Y}(\omega_m) + \widehat{\mathbf{C}}_{\mathbf{YZ}} \widehat{\mathbf{C}}_{\mathbf{ZZ}}^{-1} (z - \mathbf{Z}(\omega_m)), \tag{11}
$$

$$
\boldsymbol{C}_{m}(h) := h^{2} \left( \widehat{\boldsymbol{C}}_{\boldsymbol{Y}\boldsymbol{Y}} - \widehat{\boldsymbol{C}}_{\boldsymbol{Y}\boldsymbol{Z}} \widehat{\boldsymbol{C}}_{\boldsymbol{Z}\boldsymbol{Z}}^{-1} \widehat{\boldsymbol{C}}_{\boldsymbol{Y}\boldsymbol{Z}}^{T} \right).
$$
 (12)

It follows that the posterior PDF of Z is estimated for each  $z$  in  $\mathbb{R}^{d_z}$  by:

$$
f_{\mathbf{Z}|S(N)}(z) \approx \frac{\widehat{\mathcal{L}}_{\mathcal{S}(N)}(z;h)f_{\mathbf{Z}}(z)}{\mathbb{E}\left[\widehat{\mathcal{L}}_{\mathcal{S}(N)}(\mathbf{Z})\right]}, \quad \widehat{\mathcal{L}}_{\mathcal{S}(N)}(z;h) := \prod_{n=1}^{N} \widehat{f}_{\mathbf{Y}(z)}(\mathbf{Y}^{\star}(\theta_{n});h). \tag{13}
$$

Remarks

- $-$  One key step of these methods is the exploration of the whole space of the  $$ input variables. To maximize this overing, it is generally worth hoosing  $\{Z(\omega_1), \ldots, Z(\omega_M)\}\$ as a space filling design of experiments that preserves good projection properties for each scalar input (see [\[Fang](#page-23-13) and Lin, 2003, Fang et al., [2006,](#page-23-14) Perrin and [Cannamela,](#page-24-15) 2017 for the construction of such designs when prior density  $f_{\mathbf{Z}}$  is uniform or not).
- Another crucial aspect of these Bayesian approaches is the choice of prior distribution  $f_Z$ . Indeed, the more informative it is, the less measurements we need to get a useful posterior distribution for  $Z$ . But if it is overconfident around values that are potentially biased, the uncertainty carried by the posterior distribution may not be large enough to adequately capture the true value of  $Z$  (see [Marin and [Robert,](#page-24-16) 2007] for more details on the onstru
tion of this prior distribution).
- In the standard case, the  $M$  code evaluations are generally used to construct a surrogate model of a computationally expensive but deterministic code. Hence, depending on the dimension of the input space and the regularity of the ode output with respe
t to the inputs, interesting approximations an be obtained using relatively small values of M [\[Perrin](#page-24-17) et al., 2017]. On the contrary, in our case, as  $z \mapsto g(X(z))$  is a stochastic simulator, the value of  $M$  is likely to be higher, as we want the ode evaluations to allow a pre
ise approximation of the dependen
e stru
 ture between  $Y(Z)$  and Z in the construction of their joint PDF. And the higher  $d_y + d_z$  is, the higher value of M we may need. However, when confronted to expensive simulators, the maximal number of code evaluations is generally limited  $(M \text{ must be less than } 1000 \text{ for instance}).$  In that case, it is parti
ularly important to work on methods that allow the most pre
ise identification of the parameters at the minimal cost. This is the objective of the following sections. In Section [2.3,](#page-7-0) we first propose to decompose  $Y(Z)$ in several groups to improve the relevance of the nonparametric representation of PDF  $f_{Y,Z}$  for a fixed value of M. Then, selection criteria are proposed in Se
tion [2.5](#page-9-0) to sequentially on
entrate the ode evaluations in the most likely regions for  $Z$ , and therefore reduce the uncertainties on its posterior PDF  $f_{\mathbf{Z}|\mathcal{S}(N)}$ .

#### <span id="page-7-0"></span>2.3 Optimal partitioning

As it is explained in [\[Perrin](#page-25-6) et al., 2018], when  $d_y$  becomes high, separating in different groups the components of  $Y(Z)|Z$  that could reasonably be considered as independent can strongly improve the relevance of  $f_{\boldsymbol{Y}(\boldsymbol{z})}$  for a fixed

number of code evaluations. Let  $\boldsymbol{b} = (b_1, \ldots, b_{d_y})$  be a particular group decomposition of  $Y(Z)|Z$  in the sense that:

- if  $b_i = b_j, Y_i(\mathbf{Z})|\mathbf{Z}$  and  $Y_j(\mathbf{Z})|\mathbf{Z}$  are supposed to be dependent and therefore belong to the same blo
k,
- $i =$  if  $b_i \neq b_j ,$   $Y_i({\boldsymbol{Z}}) | {\boldsymbol{Z}}$  and  $Y_j({\boldsymbol{Z}}) | {\boldsymbol{Z}}$  are supposed to be independent and they can belong to two different blocks.

To avoid redundancies in this block by block representation, vector  $\boldsymbol{b}$  can be hosen in the set:

$$
\mathbb{B}(d_y) := \left\{ \mathbf{b} \in \{1, \dots, d_y\}^{d_y} \mid b_1 = 1, \ 1 \le b_j \le 1 + \max_{1 \le i \le j-1} b_i, \ 2 \le j \le d_y \right\}.
$$
\n(14)

Hence, for any **b** in  $\mathbb{B}(d_y)$ , we can define

- $-$  Max $(b)$  as the maximal value of  $b$ ,
- $Y^{(\ell)}(\bm{z},\bm{b})$  as the random vector that gathers all the components of  $\bm{Y}(\bm{Z})|\bm{Z}=0$  $z$  with a block index equal to  $\ell$ ,
- $-\,\, y^{(\ell)}(y,b)$  as the vector that gathers all the components of  $y$  with a block index equal to  $\ell$ .

For all **b** in  $\mathbb{B}(d_y)$ , z in  $\mathbb{R}^{d_z}$  and  $h := (h_1, \ldots, h_{\text{Max}}(b))$  in  $\mathbb{R}^{\text{Max}}(b)$ , if  $\widehat{f}_{\boldsymbol{Y}^{(\ell)}(\boldsymbol{z},\boldsymbol{b})}(\boldsymbol{y}^{(\ell)}(\boldsymbol{y},\boldsymbol{b});h_\ell)$  is the kernel estimator of the PDF of  $\boldsymbol{Y}^{(\ell)}(\boldsymbol{z},\boldsymbol{b}),$  it omes:

<span id="page-8-0"></span>
$$
f_{\mathbf{Y}(\boldsymbol{z})}(\boldsymbol{y}) \approx \widetilde{f}_{\mathbf{Y}(\boldsymbol{z})}(\boldsymbol{y};\boldsymbol{h},\boldsymbol{b}) := \prod_{\ell=1}^{\text{Max}(\boldsymbol{b})} \widehat{f}_{\mathbf{Y}^{(\ell)}(\boldsymbol{z},\boldsymbol{b})}(\boldsymbol{y}^{(\ell)}(\boldsymbol{y},\boldsymbol{b});h_{\ell}), \ \boldsymbol{y} \in \mathbb{R}^{d_y}, \quad (15)
$$

leading to another approximation of  $f_{\mathbf{Z}|{\mathcal{S}}(N)}(z)$  for each  $z$  in  $\mathbb{R}^{d_z}$ :

$$
f_{\mathbf{Z}|S(N)}(z) \approx \widetilde{f}_{\mathbf{Z}|S(N)}(z) := \frac{\widetilde{\mathcal{L}}_{\mathcal{S}(N)}(z; \mathbf{h}, \mathbf{b}) f_{\mathbf{Z}}(z)}{\mathbb{E}\left[\widetilde{\mathcal{L}}_{\mathcal{S}(N)}(\mathbf{Z})\right]},\tag{16}
$$

$$
\widetilde{\mathcal{L}}_{\mathcal{S}(N)}(\boldsymbol{z};\boldsymbol{h},\boldsymbol{b}):=\prod_{n=1}^{N}\widetilde{f}_{\boldsymbol{Y}(\boldsymbol{z})}(\boldsymbol{Y}^{\star}(\theta_{n});\boldsymbol{h},\boldsymbol{b}).
$$
\n(17)

#### 2.4 Estimation of the kernel parameters

To evaluate  $\mathcal{L}_{\mathcal{S}(N)}$ , the values of  $h$  and  $b$  have to be identified. This can be done by solving the following optimization problem:

$$
(\boldsymbol{h}^{\text{AIC}}, \boldsymbol{b}^{\text{AIC}}) \approx \arg\min_{\boldsymbol{h}\in]0,+\infty[\text{Max}(\boldsymbol{b}),\ \boldsymbol{b}\in\mathbb{B}(d_y)} \text{AIC}^{\text{LOO}}(\boldsymbol{h},\boldsymbol{b}),\tag{18}
$$

$$
\text{AIC}^{\text{LOO}}(\boldsymbol{h},\boldsymbol{b}) := 2\text{Max}(\boldsymbol{b}) - 2\log\left(\prod_{m=1}^{M}\prod_{\ell=1}^{\text{Max}(\boldsymbol{b})}\widetilde{f}_{\boldsymbol{Y}^{(\ell)}(\boldsymbol{Z}(\omega_m),\boldsymbol{b})}(\boldsymbol{Y}^{(\ell)}(\boldsymbol{Y}(\omega_m),\boldsymbol{b});h_{\ell})\right),\tag{19}
$$

where  $\hat{f}^{(-m)}_{\mathbf{Y}^{(\ell)}(\mathbf{Z}(\omega_m),\boldsymbol{b})}$  is the kernel estimator of the PDF of  $\mathbf{Y}^{(\ell)}(\mathbf{Z}(\omega_m),\boldsymbol{b})$  that is based on all the evaluations of g but the  $m<sup>th</sup>$  one. Indeed, given Eq. [\(9\)](#page-6-0), this amounts to minimizing a "Leave-One-Out" version of the Akaike information criterion (AIC) [\[Akaike,](#page-23-17) 1974] associated with the PDF of  $Y(Z)|Z$  (very close results would be obtained by considering another information criterion such as the Bayesian information criterion  $(BIC)$ ). We refer to [\[Perrin](#page-25-6) et al., 2018] for more details about the solving of this optimization problem.

#### <span id="page-9-0"></span>2.5 Adaptive strategy

By construction, the precision of the estimation of  $z^*$  depends on the number of experimental measurements,  $N$ , and the number of code evaluations, M. Classically, the value of N is fixed, whereas it should be possible to improve the accuracy of  $f_{\boldsymbol{Y}(\boldsymbol{z})}$ , which is defined by Eq. [\(15\)](#page-8-0), by adding new code evaluations in the learning set. For instance,  $M^{new}$  new points could be added to the learning set by evaluating the code in  $M^{new}$  independent realizations of  $Z|S(N)$  (we remind that no code evaluations are required to choose these new points). However, as the kernel density estimator is based on the post-pro
essing of independent and identi
ally distributed realizations of the random vector to model, non consistent results could be obtained by mixing realizations of  $\mathbf{Z}|\mathcal{S}(N)$  with realizations of  $\mathbf{Z}$ . If such a selection criterion was chosen, this would mean that the  $M$  code evaluations at the initial step should not be used for the refining.

As an alternative, we propose to evaluate the function

$$
\boldsymbol{z}\mapsto\widetilde{f}(\boldsymbol{z}):=\widetilde{\mathcal{L}}_{\mathcal{S}(N)}(\boldsymbol{z};\boldsymbol{h}^{\mathrm{AIC}},\boldsymbol{b}^{\mathrm{AIC}})f_{\boldsymbol{Z}}(\boldsymbol{z})
$$

in each value of  $\{Z(\omega_1), \ldots, Z(\omega_M)\}\)$ . For each  $1 \leq m \leq M$ , let  $\pi_m$  be the following weights:

$$
0 \le \pi_m := \frac{\widetilde{f}(\mathbf{Z}(\omega_m))}{\sum_{m'=1}^M \widetilde{f}(\mathbf{Z}(\omega_{m'}))} \le 1.
$$
\n(20)

Without loss of generality, these weights are assumed to be sorted in de creasing order,  $\pi_1 \geq \pi_2 \geq \ldots \geq \pi_M$ . Hence, for  $0 < \alpha < 1$ , if we denote by  $Q_\alpha$ the smallest integer su
h that:

<span id="page-9-1"></span>
$$
\sum_{m=1}^{Q_{\alpha}-1} \pi_m \ge \alpha,\tag{21}
$$

the domain  $\mathcal{Z}_{\alpha} := \{ \boldsymbol{z} \in \mathbb{R}^{d_z} \mid \widetilde{f}(\boldsymbol{z}) \geq \widetilde{f}(\boldsymbol{Z}(\omega_{Q_\alpha}) \}$  can be seen as a conservative  $\alpha$ -credible set for  $\mathbf{Z}|\mathcal{S}(N)$ , in the sense that the probability for  $\mathbf{Z}|\mathcal{S}(N)$  to be in  $\mathcal{Z}_{\alpha}$  is likely to be higher than  $\alpha$ . Therefore, adding new realizations of  $\mathbf{Z}|\mathbf{Z} \in \mathcal{Z}_{\alpha}$  seems a good mean to enrich the set of points on which the kernel density estimator is based. Indeed, the most likely values of  $z$  at the former step are kept in the adaptive pro
edure, while a good exploration of the input domain is expected if the value of  $\alpha$  is chosen sufficiently high.

Finally, choosing  ${f}_{Z|Z\in\mathcal{Z}_{\alpha}}$  instead of  $f_Z$  for the prior distribution of  $Z,$ and repeating several times this procedure, it is possible to iteratively reduce the uncertainties about  $z^*$ .

#### Remarks

- $-$  By adding new code evaluations, the objective is to make  $f_{\boldsymbol{Y}(\boldsymbol{z})}$  be as close to  $f_{\boldsymbol{Y}(\boldsymbol{z})}$  as possible, such that the approximate posterior  $f_{\boldsymbol{Z}|{\mathcal{S}(N)}}$  is as close to the true (but unknown) posterior  $f_{\mathbf{Z}|S(N)}$  as possible. Choosing a value of  $\alpha$  that is strictly inferior to one only aims at limiting the number of new code evaluations that will be in the region where true posterior  $f_{\boldsymbol{Z}|{\mathcal{S}(N)}}$  is almost zero. However, this value has not to be hosen too small, as it would artificially reduce the uncertainty associated with the estimation of  $z^*$  by utting too mu
h the tails of the true posterior. Hen
e, in the appli
ations that will be presented in Section [3,](#page-10-0)  $\alpha$  is chosen equal to 0.99.
- According to Eq. [\(21\)](#page-9-1), we deliberately add one to the value of  $Q_{\alpha}$  to be conservative for the estimation of the  $\alpha$ -credible set. This is particularly important for cases when after the first iteration,  $\pi_1 \approx 1$ . Indeed, even if one value of z appears to be mu
h more relevant than the others, we do not want to focus too much around a single mode.

#### <span id="page-10-0"></span>3 Appli
ations

The purpose of this section is to illustrate the method proposed in Section [2](#page-3-0) on two appli
ations.

#### <span id="page-10-1"></span>3.1 Analyti
al appli
ation

In this first application,  $X(z)$  refers to the Gaussian random fields whose mean is equal to  $t \mapsto \sin(2\pi z_3t + z_4)$ , and whose covariance function is equal to  $(t, t') \mapsto z_1^2 \exp \left(-\frac{(t-t')^2}{2z_2^2}\right)$  $2z_2^2$ .

This lass of random elds is therefore parameterized by four quantities: two parameters for the mean value, denoted by  $z_3$  and  $z_4$ , and two parameters for the covariance function, denoted by  $z_1$  and  $z_2$ . We then introduce  $U(X(z))$ as the image of  $X(z)$  by the following nonlinear mapping:



<span id="page-11-0"></span>Fig. 1 Comparison of independent realizations  $U(X(Z))$  and  $U(X(Z))|Z=z^*$ .

$$
U(X(z)) := \{ X(t; z) \sin(X(t; z)), \ t \in [0, 1] \}.
$$
 (22)

The value of  $z^*$  is chosen equal to  $(0.3, 0.2, 2, 1)$ , and it is a priori modeled by a uniformly distributed over  $[0.1, 1] \times [0.05, 1] \times [1, 3] \times [0, 2]$  random vector, denoted by Z. To identify  $z^*$ , the available information is made of  $N = 10$ independent realizations of  $U(X(\mathbf{Z}))|\mathbf{Z} = \mathbf{z}^{\star}$ , denoted by  $U^{\star}(\theta_1), \ldots, U^{\star}(\theta_N)$ . To solve the inference problem,  $M = 500$  independent realizations of Z have been drawn, which we write  $\{Z(\omega_1), \ldots, Z(\omega_M)\}\)$ . For each  $1 \leq m \leq M$ , we then draw at random one realization of  $U(X(\mathbf{Z}(\omega_m)))$ , and we denote it by  $U(\omega_m)$  for the sake of simplicity. As an illustration, several realizations of  $U(X(\mathbf{Z}))$  and  $U(X(\mathbf{Z}))|\mathbf{Z} = \mathbf{z}^*$  are compared in Figure [1.](#page-11-0)

In principle, the Bayesian formulation can be applied to any multi-variate output ode. But in pra
ti
e, it is generally very onvenient to ondense (if it is possible) the statisti
al ontent of the ode output in a low-dimensional vector [\[Perrin,](#page-24-18) ress]. In our context, it is even more important, as a key step of the proposed method is the identi
ation of the joint distribution between the parameters to be identified and the associated code output, whose complexity strongly increases with the dimension of the code output. In that prospect, we introduce  $\psi_p, p \geq 1$  as the solutions of the following eigenvalue problem:

$$
\int_0^1 \sum_{m=1}^M U(t,\omega_m)U(t',\omega_m)\psi_p(t')dt' = \lambda_p \psi_p(t),\tag{23}
$$

$$
\lambda_1 \ge \lambda_2 \ge \cdots \to 0, \int_0^1 \psi_p(t') \psi_q(t') dt' = \delta_{pq}, \tag{24}
$$

where  $\delta_{pq}$  is the Kronecker symbol that is equal to 1 if  $p = q$  and 0 otherwise. To solve the inference problem, we finally introduce  $Y(z)$  as the vector gathering the projection coefficients of  $U(X(\mathbf{Z}))$  on the former eigenfunctions associated with the  $d<sub>u</sub>$  highest eigenvalues:

$$
\boldsymbol{Y}(\boldsymbol{Z}) := \left(\int_0^1 U(t; X(\boldsymbol{Z})) \psi_1(t) dt, \dots, \int_0^1 U(t; X(\boldsymbol{Z})) \psi_{d_y}(t) dt\right). \tag{25}
$$

The value of  $d_y$  can then be chosen to guarantee a relevant representation of the observations. To this end, we introduce  $\varepsilon^2$  as the following quantity:

<span id="page-12-0"></span>
$$
\varepsilon^{2}(d_{y}) := \frac{\sum_{n=1}^{N} \int_{0}^{1} \left( U^{\star}(t, \theta_{n}) - \widehat{U}^{\star}(t, \theta_{n}; d_{y}) \right)^{2} dt}{\sum_{n=1}^{N} \int_{0}^{1} \left( U^{\star}(t, \theta_{n}) \right)^{2} dt},
$$
\n(26)

$$
\widehat{U}^{\star}(t,\theta_n;d_y) := \sum_{p=1}^{d_y} \psi_p(t) \left( \int_0^1 U^{\star}(t',\theta_n) \psi_p(t')dt' \right). \tag{27}
$$

As an illustration, Figure [2](#page-13-0) shows the evolution of  $\varepsilon^2(d_y)$  with respect to  $d_y$ , as well as the difference between  $U^*(t, \theta_1)$  and  $\widehat{U}^*(t, \theta_1; d_y)$  for three values of  $d_y$ . For this application,  $d_y$  was chosen equal to 12, which corresponds to a value of  $\varepsilon^2$  that is less than 1%.

Based on these M realizations of  $(Y(Z), Z)$ , and on these N realizations of  $\bm{Y}(\bm{z}^{\star}):=\bm{Y}(\bm{Z})|\bm{Z}=\bm{z}^{\star},$  the adaptive Bayesian formalism presented in Section [2](#page-3-0) is now applied. For this application, the parameter  $\alpha$ , which was introduced in Se
tion [2.5,](#page-9-0) is hosen equal to 0.99. At ea
h iteration, new samples are therefore added in the region where  $f_{\boldsymbol{Z}|\mathcal{S}(N)}$  is not too small using a rejection approa
h until we get a total of M points (in
luding the points omputed at the former iterations) in the  $\alpha$ -credible set  $\mathcal{Z}_{\alpha}$ , whose definition is also given in Se
tion [2.5.](#page-9-0) After 5 iterations, the total number of alls to the ode is equal to 2300, whi
h means that around <sup>450</sup> new points have been added at ea
h iteration. The results are summarized in Table [3.1](#page-13-0) and Figures [3](#page-14-0) and [4.](#page-14-1) As a first comment, we verify that the identification of  $z^*$  after only one iteration is not very pre
ise, in the sense that the predi
tion un
ertainties are very high. This is not surprising, as we are trying to approximate the PDF of a 16-dimensional random vector  $(d_y = 12, d_z = 4)$  on its whole definition domain from only 500 realizations. Moving from  $M = 500$  to  $M = 2300$ , that is to say spending the total budget at the first iteration, does not really help. Indeed, the results we get in terms of mean and variance of  $\mathbb{Z}|\mathcal{S}(N)|$ are approximatively the same. This is explained by the fact that even if the number of points is almost multiplied by five, the coverage of the definition



<span id="page-13-0"></span>Fig. 2 Evolution of the projection error with respect to  $d_y$ .

	$Z_1$	Z	$Z_3$	$Z_4$
Reference	0.3	0.2	2	1.
$\mathbb{E}[Z \mathcal{S}(N)]$ , $M = 2300$ , $i = 1$	0.25	0.57	2.00	1.02
$\mathbb{E}[Z \mathcal{S}(N)]$ , $M = 500$ , $i = 1$	0.24	0.59	2.00	1.02
$\mathbb{E}[Z \mathcal{S}(N)]$ , $M = 500$ , $i = 2$	0.35	0.31	2.00	1.04
$\mathbb{E}[Z \mathcal{S}(N)]$ , $M = 500$ , $i = 3$	0.34	0.23	2.00	1.04
$\mathbb{E}[Z \mathcal{S}(N)], M = 500, i = 4$	0.34	0.24	2.00	1.04
$\mathbb{E}[Z \mathcal{S}(N)]$ , $M=500$ , $i=5$	0.29	0.19	2.00	1.04

Table 1 Evolution of the posterior mean with respect to the iteration number.

domain stays very sparse. On the ontrary, adding iteratively around 450 new ode evaluations in the most likely region, whose volume is mu
h smaller than the initial volume, allows  $\mathbb{E}\left[\mathbf{Z}|\mathcal{S}(N)\right]$  to tend to  $\boldsymbol{z}^{\star},$  and strongly reduces the redible intervals. This onvergen
e is qui
ker for the mean parameters than for the covariance parameters, which was also expected, as the mean function is generally easier to identify than the ovarian
e. Fo
using on Figure [4,](#page-14-1) it is also interesting to noti
e that the referen
e value does not need to be in the 99%-credible ellipse associated with  $\mathbf{Z}|\mathcal{S}(N)$  at the first iteration to be in the 99%redible ellipses at the next iterations.





Fig. 3 Evolution of the 99%-credible intervals and of the mean values of the components of  $\mathbf{Z}|\mathcal{S}(N)$  with respect to the iteration number.

<span id="page-14-0"></span>

<span id="page-14-1"></span>Fig. 4 Evolution of the 99%-credible ellipses of the two first elements of  $\mathbf{Z}|\mathcal{S}(N)$  with respe
t to the iteration number.

<span id="page-14-2"></span>3.2 Application to the identification of the mechanical properties of an unknown anisotropi material

The second application deals with the identification of the mechanical properties of an heterogeneous micro-structure, which is modeled by a random elastic medium. To this end, several experimental tests are performed on a series of specimens made of the same material. To be coherent with the notations in-troduced in Section [2,](#page-3-0) we denote by  $X$  the elasticity field characterizing the



(b) Evolution of the Young modulus

2.05E+02 2.05E+02 2.06E+02 2.07E+02 2.07E+02 2.08E+02

<span id="page-15-0"></span>Fig. 5 One potential spatial variation of the Young modulus and the Poisson ratio associated with the stochastic model  $X(z^{\star}).$ 



<span id="page-15-1"></span>Fig. 6 Representation of the studied mechanical phenomenon.

mechanical properties of the material that constitutes the specimens. Several sto
hasti models have been proposed in the framework of the heterogeneous anisotropic linear elasticity [\[Soize,](#page-25-20) 2006[, Soize,](#page-25-21) 2008, Clouteau et al., 2013, Guilleminot and Soize, 2013]. It should be noted that the elasticity field is not a real-valued random field, but a tensor-valued random field, and that the different components of this random field cannot be identified separately due to algebraic constraints. For this application, the stochastic model for the elasticity field is based on the model proposed in [\[Soize,](#page-25-20) 2006] and [\[Guilleminot](#page-23-19) and Soize, 2013] in 2D plan stresses for the sake of simplicity. Hence, the distribution of  $X$  is non-Gaussian, and it is parameterized by a 5-dimensional deterministic vector  $\boldsymbol{z} = (z_1, \ldots, z_5)$ , where:

- $z_1$  is a positive dispersion coefficient that controls the level of fluctuations,
- $z_2, z_3$  are two spatial correlation lengths,
- $z_4$  is the mean value of the Young Modulus ( $\times 10^9$  Pa);
- $-z_5$  is the mean value of the Poisson ratio.

We then assume that  $N = 100$  cubic specimens are available, whose respective mechanical properties are characterized by one particular realization of  $X(z^*)$ , with  $z^* = (2000, 0.1, 0.15, 210, 0.3)$  $z^* = (2000, 0.1, 0.15, 210, 0.3)$  $z^* = (2000, 0.1, 0.15, 210, 0.3)$ . As an illustration, Figure 5 shows, for one particular specimen, the evolution of the Young modulus and the Poisson ratio in each point of  $[0,1]^2$ . The same pressure field  $\bm{f}_S = -f_S\bm{e}_2$ is then imposed on the top of each specimen, and we only have access to the induced displacement field on the boundaries of these specimens (see Figure  $6$  for an illustration of the experimental protocol). Let  $\bm{U}^{\star}(\theta_1),\ldots,\bm{U}^{\star}(\theta_N)$  be these measured displa
ements.

Based on this set of measurements, the method described in Section [2](#page-3-0) could directly be applied to the identification of  $z^*$ . To speed up this identification, following the works achieved in [\[Nguyen](#page-24-19) et al., 2015], we propose an alternative method, which is based on a two-step procedure. First,  $z_4^{\star}$  and  $z_5^{\star}$  will be identified by confronting the measured displacements to the homogeneous case. Once  $z_4^\star$  and  $z_5^\star$  have been found, a Bayesian formalism will be proposed for the identification of the three remaining components of  $z^*$ .

Indeed, if the specimens were made of a homogeneous material, characterized by its young modulus E and its Poisson ratio  $\nu$ , it is well known [Lai et al., 2010] that the induced displacement in each point  $s \in [0,1]^2$  would be equal to  $\boldsymbol{u}^{\text{homo}}(\boldsymbol{s}) = (as_1,bs_2), \text{ with}$ 

$$
\begin{pmatrix} a \\ b \end{pmatrix} = \begin{bmatrix} \lambda & \lambda + 2\mu \\ \lambda + 2\mu & \lambda \end{bmatrix}^{-1} \begin{pmatrix} 0 \\ -f_S \end{pmatrix}, \quad \mu = \frac{E}{2(1+\nu)}, \quad \lambda = \frac{2\mu\nu}{(1-2\nu)}. \tag{28}
$$

Hen
e, as we are onsidering a lass of stationary random pro
esses, the values of  $z_4^{\star}$  and  $z_5^{\star}$  can be identified as the arguments that minimize the L2 distance between the N measured displacements and the associated homogeneous displacements. In this two-step approach, the Bayesian identification is no longer arried out in dimension 5, but in dimension 3. This strongly redu
es the number of code evaluations that will be needed for a correct identification of  $(z_1^*, z_2^*, z_3^*)$ .

Thus, in the following, only  $z_1^{\star}, z_2^{\star}$  and  $z_3^{\star}$  are modeled by random quantities. They are gathered in the vector  $Z$ , whose components are assumed independent and distributed according to the following distributions:

<span id="page-17-0"></span>
$$
\log(Z_1) \sim \mathcal{U}(4.6, 11.5), \ Z_2 \sim \mathcal{U}(0.01, 0.3), \ Z_3 \sim \mathcal{U}(0.01, 0.3), \tag{29}
$$

where for all  $a < b$ ,  $\mathcal{U}(a, b)$  is the uniform distribution over [a, b]. For a given value of  $Z$ , it is possible to simulate independent realizations of  $X(Z)$ , and to approximate (using the Finite Element Method) the displa
ements indu
ed by the experimental force field, which we write  $U(X(Z))$ . Thus, for this second application, we first chose at random  $M = 1000$  values of Z according to its prior distribution. For each of these values, a particular realization of the elasticity tensor was then generated over  $[0,1]^2$ , and the mechanical problem that orresponds to the experimental proto
ol was solved (using the software Cast3M) to get the displacements at the boundary of the cube. In the same manner than in Section [3.1,](#page-10-1) we finally introduce  $Y(Z)$  as the projection of  $U(X(Z))$  on the  $d<sub>y</sub>$  first eigenfunctions associated with the empirical estimation of the covariance of  $U(X(Z))$  based on the M code evaluations. In the same manner, we gather in  $\mathcal{S}(N)$  the projection coefficients of each measured displacement  $\boldsymbol{U}^{\star}(\theta_{n})$  on this reduced basis. To choose the value of  $d_{y}$ , the normalized error defined by Eq. [\(26\)](#page-12-0) is once again considered. For this application,  $d_y$  is chosen equal to 23 in order to correctly represent most of the local oscillations of the displacements. According to Figure [7,](#page-18-0) this corresponds to a projection error that is less than  $0.1\%$ .

Following the framework proposed in Section [2,](#page-3-0) the PDF of  $\mathbb{Z}|\mathcal{S}(N)$  is deduced from the kernel estimator of the PDF of  $(Y(Z), Z)$ . An adaptive procedure (with  $\alpha = 0.99$ ) is moreover introduced to better concentrate the distribution of  $\mathbf{Z}|\mathcal{S}(N)$  on the true value of  $z^*$ . To be more precise, 900 new code evaluations were added between the two first iterations, and 620 between the two last iterations, leading to a total budget of 2520 ode evaluations. The relevance of this approach is shown in Figure [8,](#page-19-0) where the blue continuous lines correspond to the 95%-credible ellipses associated with the distribution of  $\mathbf{Z}|\mathcal{S}(N)$ . After three iterations, the values of  $z_1^{\star}, z_2^{\star}$  and  $z_3^{\star}$  are indeed identified with a high precision. To emphasize the interest of the partitioning pre-sented in Section [3.2,](#page-14-2) these results are compared to the case where there is no optimization of the blo
k stru
ture (the ellipses in red dotted lines). Although these two approa
hes are based on the same information, there is no denying that searching groups of independent components of  $Y(Z)|Z$  is really helpful. This is especially true for the first iteration, where 23 groups of independent omponents were hosen, and for the se
ond iteration, where 8 groups of independent omponents were hosen. For the third iteration, as only 4 groups



<span id="page-18-0"></span>Fig. 7 Influence of truncation parameter  $d_y$  on the representation of the measured data.



<span id="page-19-0"></span>Fig. 8 Evolution of the 95%-credible ellipses with respect to the iteration number. Blue continuous line:  $d_y = 23$  with optimization of the block structure. Red dotted line:  $d_y = 23$ without optimization of the block structure. Green dashed line:  $d_y = 5$  without optimization of the block structure.

were chosen, introducing the partitioning does not make a big difference for the PDF identi
ation, whi
h explains the similarities between the blue and the red curves.

This set of figures also emphasizes the importance of considering a high value of  $d_y$ , even if it complicates the PDF identification. For instance, choosing  $d_u = 5$  leads to the results in green dashed lines, which are clearly less relevant than the results in blue that correspond to  $d_y = 23$ . Intermediate results were obtained for values of  $d_y$  between 5 and 23, whereas still increasing  $d_y$  did not really hange the results.

In order to emphasize the efficiency of the proposed method to recover the true underlying stochasticity, three additional batches of  $Q = 10^4$  simulations are launched. These simulations are associated with the same cubic system than in Figure [6,](#page-15-1) but with different boundary conditions (by changing the boundary conditions, we want to verify that the identified values of Z are not dependent of a fixed configuration). While the boundary conditions on the inferior side of the ube do not hange, the left and right sides are now free of onstraints, and the displa
ements on the superior side are chosen equal to  $0.002e_1 - 0.01e_2$ . We then denote by  $\left\{ \boldsymbol{X}^{(1,q)}, 1 \le q \le Q \right\}$ ,  $\left\{ \boldsymbol{X}^{(2,q)}, 1 \leq q \leq Q \right\}$  and  $\left\{ \boldsymbol{X}^{(3,q)}, 1 \leq q \leq Q \right\}$  the elasticity fields characterizing the material properties of the dierent ubes of the three sets respe
tively. For all  $1 \leq q \leq Q$ ,

- $\boldsymbol{X}^{(1,q)}$  is an independent realization of the true elasticity field,  $\boldsymbol{X}(\boldsymbol{z}^{\star});$
- $-\; X^{(2,q)}$  is an independent realization of  $X((z^{q,\text{prior}},z_4^{\star},z_5^{\star})),$  where  $z^{q,\text{prior}}$ is a realization of  $Z$ , whose distribution is given by Eq. [\(29\)](#page-17-0),
- $-\; X^{(3,q)}$  is an independent realization of  $X((z^{q,\text{post}}, z_4^\star, z_5^\star)),$  where  $z^{q,\text{post}}$  is a realization of  $\mathbf{Z}|\mathcal{S}(N)$  after the three formerly presented iterations.

For each simulation, we denote by  $\boldsymbol{U}(\boldsymbol{X}^{(i,q)}),~1\leq i\leq 3,$  the concatenation of the vertical and horizontal displacements that are induced on the left and right sides of the ube. To ompare the statisti
al information gathered in these displacements, we then compute, for each  $1 \leq i \leq 3$ , the eigenvalues  $\left\{v_j^{(i)}, j \geq 0\right\}$  associated with the empirical estimate of their covariance matrices. In addition, we denote by  $\sigma^{\text{VM}}(\boldsymbol{X}^{(i,q)})$  the maximum value over the cubic domain of the Von Mises stress. This Von Mises criterion is commonly used to characterize the resistance of the system (see [Lai et al., 2010] for more details). The de
rease of these eigenvalues and the PDF of these Von Mises criteria are finally compared in Figure [9.](#page-21-0) Looking at these figures, we see that the results associated with the posterior distribution of **Z** are very close to the ones associated with the true elasticity field, which is not true for the results associated with the prior distribution of  $Z$ . This underlines the capacity of the proposed method to take into account indirect observations for the identifica-



<span id="page-21-0"></span>Fig. 9 Representation of the eigenvalues decreases (a) and of the PDFs of the Von Mises criteria (b) for the three compared configurations. In each figure, the blue continuous lines are associated with the reference case, the red dashed line correspond to the results associated with the prior distribution of Z, when the black two-dashed lines correspond to the results associated with the posterior distribution of  $\boldsymbol{Z}.$ 

tion of the parameters characterizing the distribution of an unknown random pro
ess of interest.

## 4 Con
lusion

The in
reasing of the omputational resour
es and the generalization of the monitoring of mechanical systems have encouraged many scientific fields to take into account random fields in their modeling. In that prospect, this work proposes an adaptive Bayesian framework to efficiently identify the statistical properties of these random fields when the available information is a reduced set of indirect observations. Two examples based on simulated data are finally presented to show the potential of this approa
h.

Extending this approach to the cases where the number of parameters to identify and the number of observations are very high would be interesting for future work.

### Appendix

A.1. Proof of the equality of Eq. [9](#page-6-0)

Let  $A, B, D$  be the block decomposition matrices of  $\widehat{\boldsymbol{C}}^{-1}$ :

$$
\widehat{\boldsymbol{C}}^{-1} = \begin{bmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{B}^T & \boldsymbol{D} \end{bmatrix} . \tag{30}
$$

Using the Schur complement, if follows that:

$$
\begin{cases}\n\hat{C}_{ZZ}^{-1} = D - B^T A^{-1} B, \\
(\hat{C}_{YY} - \hat{C}_{YZ} \hat{C}_{ZZ}^{-1} \hat{C}_{YZ}^T)^{-1} = A, \\
-\hat{C}_{YZ} \hat{C}_{ZZ}^{-1} = A^{-1} B.\n\end{cases}
$$
\n(31)

It comes

$$
\begin{split}\n& \left( (\boldsymbol{y}, \boldsymbol{z}) - (\boldsymbol{Y}(\omega_m), \boldsymbol{Z}(\omega_m)) \right)^T (h^2 \hat{\boldsymbol{C}})^{-1} \left( (\boldsymbol{y}, \boldsymbol{z}) - (\boldsymbol{Y}(\omega_m), \boldsymbol{Z}(\omega_m)) \right) \\
& = \frac{1}{h^2} \begin{pmatrix} (\boldsymbol{y} - \boldsymbol{Y}(\omega_m))^T \boldsymbol{A} (\boldsymbol{y} - \boldsymbol{Y}(\omega_m)) + 2(\boldsymbol{y} - \boldsymbol{Y}(\omega_m))^T \boldsymbol{A} \boldsymbol{A}^{-1} \boldsymbol{B} (\boldsymbol{z} - \boldsymbol{Z}(\omega_m)) \\
+ (\boldsymbol{z} - \boldsymbol{Z}(\omega_m))^T \boldsymbol{D} (\boldsymbol{z} - \boldsymbol{Z}(\omega_m))\n\end{pmatrix} \\
& = \frac{1}{h^2} \begin{pmatrix} (\boldsymbol{y} - \boldsymbol{Y}(\omega_m) + \boldsymbol{A}^{-1} \boldsymbol{B} (\boldsymbol{z} - \boldsymbol{Z}(\omega_m)))^T \boldsymbol{A} (\boldsymbol{y} - \boldsymbol{Y}(\omega_m) + \boldsymbol{A}^{-1} \boldsymbol{B} (\boldsymbol{z} - \boldsymbol{Z}(\omega_m))) \\
+ (\boldsymbol{z} - \boldsymbol{Z}(\omega_m))^T \left( \boldsymbol{D} - \boldsymbol{B}^T \boldsymbol{A}^{-1} \boldsymbol{B} \right) (\boldsymbol{z} - \boldsymbol{Z}(\omega_m)) \\
= (\boldsymbol{y} - \boldsymbol{\mu}_n(\boldsymbol{z}))^T \boldsymbol{C}_n^{-1} (\boldsymbol{y} - \boldsymbol{\mu}_n(\boldsymbol{z})) + \frac{1}{h^2} (\boldsymbol{z} - \boldsymbol{Z}(\omega_m))^T \boldsymbol{C}_{\boldsymbol{Z} \boldsymbol{Z}}^{-1} (\boldsymbol{z} - \boldsymbol{Z}(\omega_m)) \\
& & (32)\n\end{split}
$$

This leads to the sear
hed result.

#### Referen
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