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A comparison between Bayesian and ordinary kriging based on validation criteria: application to radiological characterisation

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Abstract

In decommissioning projects of nuclear facilities, the radiological characterisation step aims to estimate the quantity and spatial distribution of different radionuclides. To carry out the estimation, measurements are performed on site to obtain preliminary information. The usual industrial practice consists in applying spatial interpolation tools (as the ordinary kriging method) on these data to predict the value of interest for the contamination (radionuclide concentration, radioactivity, etc.) at unobserved positions. This paper questions the ordinary kriging tool on the well-known problem of the overoptimistic prediction variances due to not taking into account uncertainties on the estimation of the kriging parameters (variance and range). To overcome this issue, the practical use of the Bayesian kriging method, where the model parameters are considered as random variables, is deepened. The usefulness of Bayesian

kriging, whilst comparing its performance to that of ordinary kriging, is demonstrated in the small data context (which is often the case in decommissioning projects). This result is obtained via several numerical tests on different toy models, and using complementary validation criteria: the predictivity coefficient (Q^2), the Predictive Variance Adequacy (PVA), the α -Confidence Interval plot (and its associated Mean Squared Error α ($MSE\alpha$)), and the Predictive Interval Adequacy (PIA). The latter is a new criterion adapted to the Bayesian kriging results. Finally, the same comparison is performed on a real dataset coming from the decommissioning project of the CEA Marcoule G3 reactor. It illustrates the practical interest of Bayesian kriging in industrial radiological characterisation.

Keywords: Geostatistics, Bayesian kriging, Ordinary kriging, Validation criteria, Radiological characterisation

1 Introduction

Radiological characterisation is one of the main challenges encountered in the nuclear industry for the decommissioning and dismantling (D&D) of old infrastructures such as buildings (see, e.g., Attiogbe et al. (2014), EPRI (2016) and CEA/DEN (2017)). Its main goal is to evaluate the quantity and spatial distribution of radionuclides. As such, measurements are made to constitute a dataset and obtain preliminary information. While measurements are made, many problems can arise. The radioactivity present on site can be dangerous for operators and does not allow for many measurements. In some extreme cases, drones and robots have to be used, making measurements more expensive and reducing the size of the datasets (see, e.g., Goudeau et al. (2015) and CEA/DEN (2017)). It is therefore quite common in nuclear D&D characterisation to have only a small number of available data: a balance has to be found between data acquisition costs and provided information from data. Statistical tools make it possible to optimise the information extracted from the data, within a rigorous mathematical framework and with associated confidence intervals (in the D&D field, see, e.g., Zaffora et al. (2016), Blatman et al. (2017) and Pérot et al. (2020)).

More precisely, as in many other environmental and industrial fields (see, e.g., Webster and Oliver (2007) and Daya Sagar et al. (2018)), spatial statistics and geostatistical methods are used to predict the variables of interest at an unobserved location (prediction of the expected value), with an indication of the expected error in prediction (prediction variance). The methodology is often based on two steps: first the construction of a statistical model with the estimation of its parameters, followed by the prediction with the statistical model for any unobserved point. The ordinary kriging model (see, e.g., Chilès and Delfiner (2012) and Cressie (1993)) is one of the most widely used models in industrial practice of D&D (see, e.g., Attiogbe et al. (2014), Goudeau et al. (2015) and EPRI (2016)). However, a common criticism is that its predictions do not take into account the uncertainty in the estimation of the model parameters. As a result, the variances of the predictions are often too optimistic and these

neglected uncertainties in the model parameters can have a significant impact. This problem is made worse for smaller datasets, which can be common in D&D projects. For the radiological characterisation in D&D projects, the first examples of kriging shown in Jeannée et al. (2008), Desnoyers (2010) and Desnoyers et al. (2011) have studied practical cases based on many measurements and did not consider this issue. The more realistic studies by Boden et al. (2013), Lajaunie et al. (2020) and Desnoyers et al. (2020), carried out on smaller datasets, have instead highlighted the errors generated by the estimation errors of the kriging parameters.

To overcome this kriging issue, a Bayesian approach was first proposed by Kitanidis (1986). Its main goal was to take into account the uncertainties in the scale and mean parameters of the kriging model. The work of Handcock and Stein (1993) then completed the full Bayesian approach which considers all the parameters of the model as unknown. More recently, a slightly different approach was presented by Krivoruchko and Gribov (2019) and is called empirical Bayesian kriging. While the equations are similar to the ones of regular Bayesian kriging, the choice on the prior distributions of kriging parameters are obtained through unconstrained simulations of the random field. This approach was adapted to allow for multi-fidelity applications, where Bayesian theory is used to update the initial data with new, more accurate data (classically used with cokriging if correlations between old and new data exist). Some examples can be found in meteorology with Gupta et al. (2017) or for oil extraction in Al-Mudhafar (2019). Note that a more complete description of Bayesian kriging with an extension to generalised linear models are presented in Diggle and Ribeiro (2007).

In this framework, our work aims to understand the usefulness of the Bayesian kriging approach, compared to the ordinary kriging one, for the radiological characterisation of contaminated buildings. In particular, the specification of a priori laws for the parameters in Bayesian kriging, which allows a more robust estimation of these parameters when only a few observations are available, is studied. The performance of ordinary and Bayesian kriging is compared on several numerical examples. For this, we not only focus on the kriging predictor accuracy but also on the kriging predictive variance accuracy. Indeed, the kriging variance is often used by practitioners to estimate confidence intervals on predicted quantities, to justify their choice of sampling, or to find locations of new (potentially expensive) measurements (Bechler et al. 2013). To ensure a certain level of confidence in the use of the predictive variance, the works of Marrel et al. (2012), Bachoc (2013a) and Demay et al. (2022), about kriging model validation, have emphasised the usefulness of several validation criteria, as the Predictive Variance Adequacy (*PVA*) and the α -Confidence Interval (α -CI) plot. In addition to allow a more accurate comparison in the case of the Bayesian kriging model, new validation criteria are required and are proposed in the present work.

The following section describes the different studied kriging models, while Section 3 develops the associate classical validation criteria before introducing the newly proposed ones. Section 4 presents the results of the model comparison

obtained on several numerical tests. Section 5 then illustrates the application on a real case study coming from the decommissioning project of the CEA Marcoule G3 reactor. Section 6 gives some conclusions.

2 The ordinary and Bayesian kriging models

This section provides reminders on kriging principles, within the framework of Gaussian random field model.

2.1 The Gaussian random field model

The variable of interest is assumed to be a random field $\{Z(\mathbf{x}), \mathbf{x} \in D\}$, with $D \subset \mathbb{R}^2$. $Z(\cdot)$ is supposed to be isotropic and stationary, meaning that

$$\forall \mathbf{x} \in D, E[Z(\mathbf{x})] = \beta,$$

$$\forall \mathbf{x}, \mathbf{x}' \in D, \text{Cov}(Z(\mathbf{x}), Z(\mathbf{x}')) = \sigma^2 C_\phi(|\mathbf{x} - \mathbf{x}'|),$$

where C_ϕ is the correlation function where $C_\phi(0) = 1$, and β, σ^2, ϕ denote the mean, variance and range (or correlation length) parameters, respectively. For ease of notation, densities will be denoted as $p(\cdot)$ and the conditioning to parameters will be simplified from $Z|\beta = \hat{\beta}$ to $Z|\beta$. The term C_ϕ corresponds to a semi-definite positive function. Moreover, by definition of a Gaussian process, every finite set of Z is a multivariate normal distribution (denoted $\mathcal{N}(\cdot, \cdot)$). Thus for n observations at positions $\mathbf{x}_1, \dots, \mathbf{x}_n$, we obtain the Gaussian random vector $Z = (Z(\mathbf{x}_1), \dots, Z(\mathbf{x}_n))'$:

$$Z|\beta, \sigma^2, \phi \sim \mathcal{N}(\beta \mathbf{1}_n, \sigma^2 \mathbf{R}_\phi),$$

where $\mathbf{1}_n$ is the vector $(1, \dots, 1)'$ of length n , and the covariance matrix is $\sigma^2 \mathbf{R}_\phi = (\text{Cov}(Z(\mathbf{x}_i), Z(\mathbf{x}_j)))_{1 \leq i, j \leq n}$. The observation sample of Z is written $\mathbf{z} = (z(\mathbf{x}_1), \dots, z(\mathbf{x}_n))'$.

The semi-definite positive function C_ϕ is often modeled using common covariance function. In this work, two covariance models will be used (see, e.g., Chilès and Delfiner (2012) for an extensive list of covariance functions). The first one is the Gaussian covariance function written

$$\forall h \in \mathbb{R}, C_\phi(h) = e^{-h^2/\phi^2},$$

while the second one is the Matérn covariance function written

$$\forall h \in \mathbb{R}, C_{\phi, \nu}(h) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu} \frac{h}{\phi} \right)^\nu K_\nu \left(\sqrt{2\nu} \frac{h}{\phi} \right), \quad (1)$$

with ν a strictly positive parameter, $\Gamma(\cdot)$ the gamma function and $K_\nu(\cdot)$ the modified Bessel function of second type and order ν . The parameter ν , that drives the regularity of the process trajectories, is not estimated. It is chosen

from a set of possible values, the most commonly used being $\nu \in \{\frac{1}{2}, \frac{3}{2}, \frac{5}{2}\}$. In addition, we have the nugget effect, written

$$\forall h \in \mathbb{R}, C_{\tau^2}(h) = \tau^2 \delta(h),$$

with τ^2 a variance and δ the Dirac function where $\delta(h) = 1$ if $h = 0$ and $\delta(h) = 0$ otherwise. The nugget effect is often used to model micro-scale variations and measurements uncertainties. In our case studies, it will only be used to improve the conditioning of the matrix \mathbf{R}_ϕ , in order to improve the stability of its numerical inversion (especially in the case of Gaussian covariance function).

The model is therefore specified by three different parameters: the trend parameter $\beta \in D_\beta$, the variance parameter $\sigma^2 \in D_{\sigma^2}$ and the range parameter $\phi \in D_\phi$. In the case of ordinary kriging and for the covariance functions considered here, the parameter spaces are

$$D_\beta = \mathbb{R}, D_{\sigma^2} =]0, +\infty[, D_\phi =]0, +\infty[.$$

The first step of the kriging methodology in practice is to estimate these parameters. Two main procedures are commonly used: variographic analysis and maximum likelihood estimation. An extensive literature is available about parameter estimation with variographic analysis, such as Chilès and Delfiner (2012) and Webster and Oliver (2007). In this work, we will use maximum likelihood estimation to take advantage of the probabilistic framework and to avoid manual or automatic fitting of variograms, especially since our numerical tests will require parameter estimation for many simulated data sets. Moreover, the automatic fitting of variograms is strongly discouraged in most of the literature (see, e.g., Chilès and Delfiner (2012) and Webster and Oliver (2007)). Note that, for the maximum likelihood estimation, an optimization algorithm with a multi-start procedure could be used to avoid the known pitfall of local extrema and better explore the parameter space. However, this procedure will not be used here because preliminary studies have shown that in our case it is not really necessary, probably due to the small dimension of the problem (2D, i.e., two-dimensional, random field) and the regularity of the likelihood function. This decision allowed to reduce computation times without compromising parameter estimation.

2.2 Kriging model principles

The kriging predictor is a linear interpolator whose expressions are derived from supplementary conditions, such as minimizing the prediction variance. For a detailed description of kriging and its construction, the reader can refer to the reference books of Chilès and Delfiner (2012), Cressie (1993) for geostatistics, but also Rasmussen and Williams (2006) for the Gaussian process regression point of view. Let \mathbf{x}_0 be an unobserved position at which we wish to predict the expected value and the variance of $Z(\mathbf{x}_0)|\sigma^2, \phi, \mathbf{Z} = \mathbf{z}$ (the mean is considered

unknown). The ordinary kriging equations are then

$$\begin{aligned}\mathbb{E}[Z(\mathbf{x}_0)|\sigma^2, \phi, \mathbf{Z} = \mathbf{z}] &= \left(\mathbf{r} + \mathbf{1}_n \frac{1 - \mathbf{1}'_n \mathbf{R}_\phi^{-1} \mathbf{r}}{\mathbf{1}'_n \mathbf{R}_\phi^{-1} \mathbf{1}_n} \right)' \mathbf{R}_\phi^{-1} \mathbf{Z}, \\ \text{Var}[Z(\mathbf{x}_0)|\sigma^2, \phi, \mathbf{Z} = \mathbf{z}] &= \sigma^2 \left(1 - \mathbf{r}' \mathbf{R}_\phi^{-1} \mathbf{r} + \frac{(1 - \mathbf{1}'_n \mathbf{R}_\phi^{-1} \mathbf{r})^2}{\mathbf{1}'_n \mathbf{R}_\phi^{-1} \mathbf{1}_n} \right),\end{aligned}$$

with $\sigma^2 \mathbf{r} = (\text{Cov}(Z(\mathbf{x}_0), Z(\mathbf{x}_j))_{1 \leq j \leq n})$.

A major concern for applications of these equations is that they are conditional on the knowledge of the variance and range parameters, which is mostly unrealistic since they are estimated. This assumption yields overoptimistic prediction variances and narrower confidence intervals. This problem is made worse in the case of a small dataset where parameter estimation is sensitive to each observation. To address this issue, more robust methods exist such as cross-validation estimation (Bachoc 2013b). Another solution is to consider the parameters as random variables. Bayesian approach seems natural in this case and leads to Bayesian kriging.

2.3 Bayesian kriging principles

Bayesian kriging deals simultaneously with estimation and predictions by considering the parameters as random variables that must be predicted conditionally to the observed data (Diggle and Ribeiro 2002). Bayesian kriging predictions are derived from the predictive distribution as follows:

$$\begin{aligned}p(Z(\mathbf{x}_0)|\mathbf{Z} = \mathbf{z}) &= \int_{D_\beta \times D_{\sigma^2} \times D_\phi} p(Z(\mathbf{x}_0), \beta, \sigma^2, \phi | \mathbf{Z} = \mathbf{z}) d\beta d\sigma^2 d\phi \\ &= \int_{D_\beta \times D_{\sigma^2} \times D_\phi} p(Z(\mathbf{x}_0) | \beta, \sigma^2, \phi, \mathbf{Z} = \mathbf{z}) p(\beta, \sigma^2, \phi | \mathbf{Z} = \mathbf{z}) d\beta d\sigma^2 d\phi \\ &= \int_{D_\phi} p(Z(\mathbf{x}_0) | \phi, \mathbf{Z} = \mathbf{z}) p(\phi | \mathbf{Z} = \mathbf{z}) d\phi.\end{aligned}$$

The density $p(Z(\mathbf{x}_0)|\phi, \mathbf{Z} = \mathbf{z})$ is known to be a Student's t -density under usual assumptions for the prior distribution (as demonstrated in Le and Zidek (1992)), but the density $p(\phi|\mathbf{Z} = \mathbf{z})$ is not an usual one, and the integral is usually intractable. In practice, it must therefore be estimated numerically. The most commonly used method for this is a Metropolis-Hasting type algorithm. More details about this algorithm can be found in Tanner (1993) and Carlin and Louis (2013). Another approach given in Tanner (1993), and used in the `geoR` package (Ribeiro and Diggle 2001) of the R software, is a Monte-Carlo approximation of the predictive distribution. This approximation is done by sampling the prior distribution of ϕ and injecting these sampled values into the density $p(Z(\mathbf{x}_0)|\phi, \mathbf{Z} = \mathbf{z})$. It should be noted that this approach is also presented in Gaudard et al. (1999), where it is applied to compare different prior choices of

ϕ distribution for modeling and predicting precipitation measurements. So, the algorithm described by Algorithm 1 will be used in the following to estimate the Bayesian prediction.

Algorithm 1 Monte-Carlo approximation for Bayesian kriging

Choose a prior specification and a prediction target \mathbf{x}_0
 Sample a value ϕ from $p(\phi|\mathbf{Z} = \mathbf{z})$
 Compute $p(Z(\mathbf{x}_0)|\phi, \mathbf{Z} = \mathbf{z})$ by injecting the sampled value ϕ
 Sample a value $z(\mathbf{x}_0)$ from $p(Z(\mathbf{x}_0)|\phi, \mathbf{Z} = \mathbf{z})$
 Reiterate the three previous steps as many times as needed to approximate the predictive distribution $p(Z(\mathbf{x}_0)|\mathbf{Z} = \mathbf{z})$
 Take $\mathbb{E}[Z(\mathbf{x}_0)|\mathbf{Z} = \mathbf{z}]$ and $Var(Z(\mathbf{x}_0)|\mathbf{Z} = \mathbf{z})$ as prediction mean and prediction variance.

As per usual in Bayesian framework, a joint prior distribution is chosen for β, σ^2 :

$$\pi(\beta, \sigma^2) \propto \frac{1}{\sigma^2}.$$

For ϕ , the prior is reduced to a uniform law between the minimum $d_{\phi, min}$ and the maximum distance $d_{\phi, max}$ allowed by the dataset:

$$\phi \sim \mathcal{U}([d_{\phi, min}, d_{\phi, max}]).$$

According to the priors thus specified, the resulting parameter space is:

$$D_\beta = \mathbb{R}, D_{\sigma^2} =]0, +\infty[, D_\phi = [d_{\phi, min}, d_{\phi, max}].$$

Note that a sensitivity analysis is presented in the Appendix (Section 7) to explain our choice of priors.

3 Validation criteria

Choosing an “optimal” covariance model for geostatistical predictions is a classical issue in geostatistics (Chilès and Delfiner 2012). It has been recently deepened in Demay et al. (2022), where interpretable validation criteria allow to assess the quality of both the predictions of the model and the associated prediction variances. The expressions of these criteria, with some new adaptations, are given in this section in their leave-one-out cross-validation form. Extension to K -fold cross-validation or to test set cases are immediate.

3.1 Predictivity coefficient (Q^2)

The main goal of this coefficient, often called “Nash-Sutcliffe criterion” (Nash and Sutcliffe 1970), is to evaluate the predictive accuracy of the model by nor-

malising the errors, allowing a direct interpretation in terms of explained variance. Its practical definition (Marrel et al. 2008) is:

$$Q^2 = 1 - \frac{\sum_{i=1}^n (z(\mathbf{x}_i) - \widehat{z}_{-i})^2}{\sum_{i=1}^n (z(\mathbf{x}_i) - \widehat{\mu})^2},$$

where \widehat{z}_{-i} is the value predicted at location \mathbf{x}_i by the model built without the i -th observation (the one located at \mathbf{x}_i) and $\widehat{\mu}$ is the empirical mean of the dataset. Its theoretical definition can be found in Fekhari et al. (2022).

The Q^2 coefficient measures the quality of the predictions and how near they are to the observed values. Its formula is similar to the coefficient of determination used for regression (with independent observations), but estimated here in prediction (by using cross-validation residuals). The closer its value is to 1, the better the predictions are (relatively to the observations). As a rule of thumb, if the Q^2 is smaller than 0.5 (i.e., less than 50% of output variance explained), the model is not considered to be good, and should be used with precaution if no other model offers better predictions.

3.2 Predictive variance adequacy (*PVA*)

This second criterion aims to quantify the quality of the prediction variances given by the kriging model. Finely studied in Bachoc (2013a;b) and Demay et al. (2022), it is defined by

$$PVA = \left| \log \left(\frac{1}{n} \sum_{i=1}^n \frac{(z(\mathbf{x}_i) - \widehat{z}_{-i})^2}{\widehat{s}_{-i}^2} \right) \right|,$$

where \widehat{s}_{-i}^2 is the prediction variance (at location \mathbf{x}_i) of the model built without the i -th observation (the one located at \mathbf{x}_i).

This coefficient estimates the average ratio between the squared observed prediction error and the prediction variance. It therefore gives an indication of how much a prediction variance is larger or smaller than the one expected. The closer the *PVA* is to 0, the better the prediction variances are. For example, a *PVA* close to 0.7 indicates prediction variances that are on average two times larger or smaller than the squared errors.

3.3 Predictive interval adequacy (*PIA*)

The *PVA* is a criterion of variance adequacy but does not take into account a possible skewness in the predictive distribution. In the Gaussian case (like ordinary kriging), mean and variance completely characterise the distribution. But in the case of Bayesian kriging where the predictive distribution is no longer Gaussian, the Q^2 and *PVA* are not sufficient to evaluate the quality of the model and its prediction. As such, we propose a new complementary geometrical criterion called the predictive interval adequacy (*PIA*) and defined as

$$PIA = \left| \log \left(\frac{1}{n} \sum_{i=1}^n \frac{(z(\mathbf{x}_i) - \widehat{z}_{-i})^2}{(\widehat{q}_{0.31,-i} - \widehat{q}_{0.69,-i})^2} \right) \right|,$$

where $\widehat{q}_{0.31,-i}$ (respectively $\widehat{q}_{0.69,-i}$) is the estimation of the quantile of order 0.31 (respectively 0.69) of the predictive distribution (at location \mathbf{x}_i) without the i -th observation.

The *PIA* has been defined to be identical to the *PVA* for a Gaussian distribution. However, rather than comparing squared errors to the predictive variance, it compares the width of prediction intervals with the squared errors. Another main difference is that the intervals considered by the *PIA* are centered on the median while those of the *PVA* are centered around the mean. Finally, an estimation of the predictive distribution is necessary to compute in practice this criterion, whereas the *PVA* only requires the computation of predictive mean and variance.

3.4 α -CI plot

The Gaussian process model allows to build prediction intervals of any level $\alpha \in]0, 1[$:

$$CI_\alpha(z(\mathbf{x}_i)) = [\widehat{z}_{-i} - \widehat{s}_{-i}q_{(1+\alpha)/2}^N; \widehat{z}_{-i} + \widehat{s}_{-i}q_{(1+\alpha)/2}^N],$$

where $q_{(1+\alpha)/2}^N$ is the quantile of order $(1 + \alpha)/2$ of the standard normal distribution. This expression is only valid if all parameters are known. For example, if the variance parameter is poorly estimated, the width of the predicted confidence intervals will not reflect what we might observe. But how can we validate a confidence interval without prior knowledge of the model parameters? The idea behind this criterion (see Marrel et al. (2012) and Demay et al. (2022)) is to evaluate empirically the number of observations falling into the predicted confidence intervals and to compare this empirical estimation to the theoretical ones expected:

$$\Delta_\alpha = \frac{1}{n} \sum_{i=1}^n \phi_i \text{ where } \phi_i = \begin{cases} 1 & \text{if } z(\mathbf{x}_i) \in CI_\alpha(z(\mathbf{x}_i)) \\ 0 & \text{else.} \end{cases}$$

This value can be computed for varying α , and can then be visualised against the theoretical values, yielding what Demay et al. (2022) calls the α -CI plot, with an example given in Figure 1.

Similarly to the *PIA*, the α -CI plot must be adapted to the Bayesian kriging since the posterior distribution is not Gaussian. We therefore introduce a slightly different criterion based on the quantiles of the predictive distribution. More precisely, this modified α -CI plot relies now on credible intervals defined as

$$\widetilde{CI}_\alpha(z(\mathbf{x}_i)) = [\widehat{q}_{\frac{1-\alpha}{2}}; \widehat{q}_{\frac{1+\alpha}{2}}],$$

where $\widehat{q}_{\frac{1-\alpha}{2}}$ (respectively $\widehat{q}_{\frac{1+\alpha}{2}}$) is the estimation of the quantile of order $\frac{1-\alpha}{2}$ (respectively $\frac{1+\alpha}{2}$) of the predictive distribution (at location \mathbf{x}_i) of the model built without the i -th observation. Once again, we obtain a criterion that is identical for both methods when the predictive distribution is Gaussian. Illustrations of α -CI plot can be found in Demay et al. (2022).

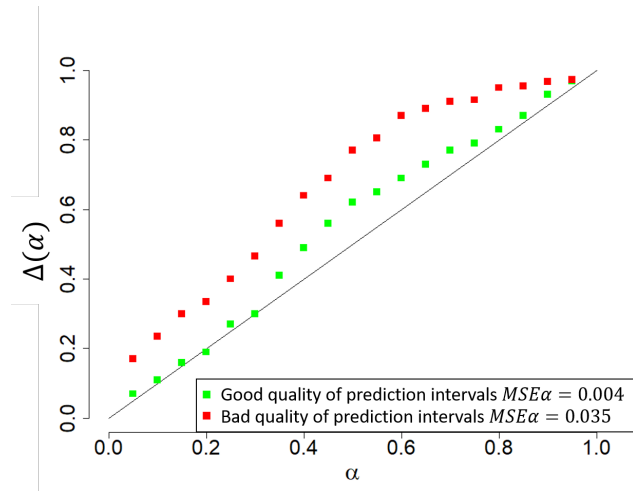


Figure 1: Example of two α -CI plots and corresponding values of $MSE\alpha$ for a good (in green) and bad (in red) predictive error model.

3.5 Mean Squared Error α ($MSE\alpha$)

Finally, to summarise the α -CI plot, we also introduce a quantitative criterion called “Mean Squared Error α ” and defined as

$$MSE\alpha = \frac{1}{n_\alpha} \sum_{j=1}^{n_\alpha} (\Delta_{\alpha_j} - \alpha_j)^2,$$

where the considered levels α are discretised over $]0, 1[$ in n_α possible values. In practice a regular discretization will be considered to compute $MSE\alpha$. The closer this criterion is to 0, the better the confidence/credible intervals are on average. To illustrate the values taken by the criterion, Figure 1 gives the α -CI plot corresponding to a “good” and “bad” model fitting.

In this graph, the bad model yields a $MSE\alpha$ of 0.035 against 0.004 for a model with more accurate prediction intervals. As a rule of thumb, a $MSE\alpha$ of 0.01 will be considered to correspond to a model with wrong predictive intervals, while a model with a $MSE\alpha$ of 0.001 will be deemed to have correct predictive intervals. Similarly to the *PVA*, the $MSE\alpha$ does not explain if the poorly fitted predictive intervals are due to badly centered predictive intervals or if the predictive variance was badly estimated (and whether or not this variance was underestimated or overestimated). This criterion must therefore be used in conjunction with the previous criteria to better assert the model qualities and weaknesses. Finally, this criterion also offers a quantitative tool for comparing different models if the α -CI plots do not allow to clearly distinguish the performances of competing models. This will be illustrated in particular in the numerical tests in Section 4.2 (Fig. 8).

The different aforementioned criteria provide complementary information to evaluate the prediction quality of the kriging model, either in terms of mean, variance or confidence/credible intervals. They will be used in the following to compare the performance of ordinary and Bayesian kriging.

4 Numerical tests and results

Our goal is to compare Bayesian and ordinary kriging (the latter being the more commonly used kriging method). To do so, the different criteria mentioned in Section 3 will be computed on datasets (i.e., samples of observations), coming from different models, of different sizes.

4.1 Datasets from 2D Gaussian process simulations

First, we consider samples simulated from an analytical Gaussian process model with known parameters. More precisely, the samples are simulated in the input space $[0, 10]^2$ from a Gaussian process with an exponential covariance (i.e., the Matérn covariance of Eq. (1) with $\nu = 0.5$) and the following parameters:

$$\beta = 0.5, \sigma^2 = 0.1, \phi = 4.5.$$

We simulate datasets of different sizes, varying from 16 to 81 observations, sampled on a square grid in the input space. Here, the sampling designs will be regular squared grids. This choice is made to comply with the application purpose which deals with D&D constraints of buildings. Indeed, most of the times, the radiological measurements inside buildings are made regularly (equidistant location) along lines of investigations (see, e.g. Attiogbe et al. (2014) and EPRI (2016)). For each size, the process is repeated 100 times with independent random Gaussian process simulations.

For each dataset, Bayesian and ordinary kriging models are estimated and the different validation criteria are computed by cross-validation. Every kriging predictions (Bayesian and ordinary) are made with the R package `geoR` (Ribeiro and Diggle 2001). Results are given in Figure 2 with boxplots (corresponding to the 100 random replicates) w.r.t. the dataset sizes. The results indicate that Bayesian kriging performs better in terms of both mean and prediction variance for small sample sizes. More precisely, Bayesian kriging outperforms ordinary kriging on all the four criteria for datasets with less than 40 observations. This result is especially visible for the *PVA* and *PIA* and shows that the main difference between both kriging methods still lies in the predictive variance accuracy. By taking into account the additional uncertainty in the estimation of the Gaussian process parameters, Bayesian kriging therefore yields larger and more accurate prediction intervals, and as a result better *PVA*, *PIA*, and *MSE α* criteria.

More precisely, if we first look at the median values of Q^2 estimation, these increase from 0 to 0.63, according to the data size, for ordinary kriging. Bayesian kriging gives better Q^2 for smaller datasets, starting from a median value of 0.16

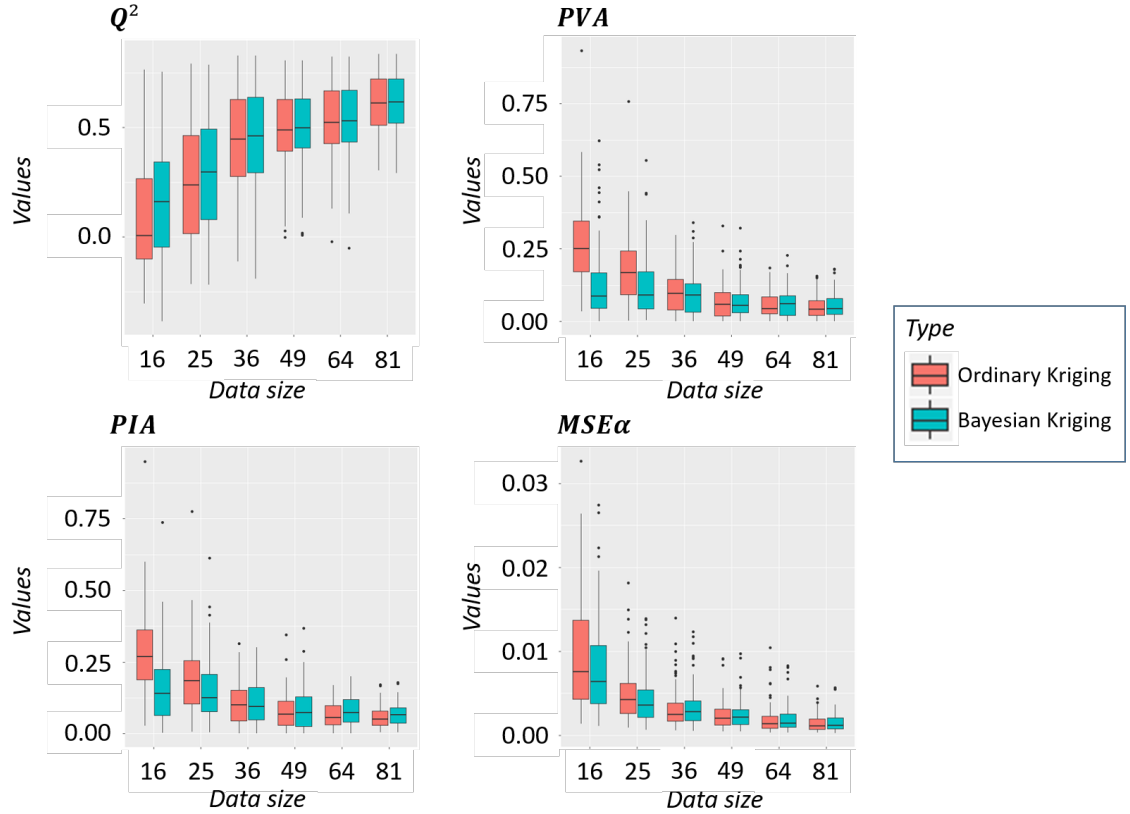


Figure 2: Distribution of validation criteria (Q^2 , PVA , PIA , and $MSE\alpha$) w.r.t. the size of datasets, for Gaussian process simulation datasets.

up to 0.63. For a fixed sample size, the dispersion of Q^2 is quite similar between both kriging methods (the geometry of sampling being fixed).

Regarding the median of PVA , the value range from 0.25 to 0.04 for ordinary kriging, compared to 0.08 to 0.04 for Bayesian kriging. For the PIA , the results are identical for ordinary kriging, but Bayesian kriging performs slightly worse, starting at 0.15 up to 0.05. We can also see that the dispersion of PIA and PVA estimates is different for small datasets between both kriging methods. This is explained by the fact that PVA and PIA are sensitive to the parameter estimation process. Since the number of observation is low, maximum likelihood estimations are not robust, yielding large variations in parameter estimations, and therefore in PVA and PIA estimations. Finally, we observe that for datasets larger or equal to 49, Bayesian kriging seems to perform slightly worse, but the differences are too small to be considered significant.

The $MSE\alpha$ graph shares similarities with the other graphs, since confi-

dence and credible intervals both depends on prediction mean and variance. For the ordinary kriging, the median $MSE\alpha$ goes from 0.0075 to 0.0025, while for Bayesian kriging the values are lower, from 0.006 to 0.0025. The evolution observed is similar between the *PVA* and *PIA*, with Bayesian kriging yielding better results for smaller datasets.

It can also be noted that for larger datasets, Bayesian and ordinary kriging yield similar results. This observation was to be expected, since Bayesian and inferential methodology coincide for larger datasets. It can therefore be argued that Bayesian kriging becomes less advantageous and relevant for datasets with more than 40 observations. Note that Q^2 values are also extremely low for 49 observations or fewer, but again this is to be expected for very small datasets.

4.2 Datasets from a 2D deterministic function

In order to test the kriging models on cases that do not fall within the theoretical framework of the Gaussian process hypothesis, we consider a sample coming from the following two-dimensional deterministic function (Iooss et al. 2010):

$$f(x, y) = \frac{e^x}{5} - \frac{y}{5} + \frac{y^6}{3} + 4y^4 - 4y^2 + \frac{7x^2}{10} + x^4 + \frac{3}{4x^2 + 4y^2 + 1}, \quad (2)$$

where (x, y) are the function inputs. Figure 3 shows this function over the $D = [-1, 1]^2$ input space.

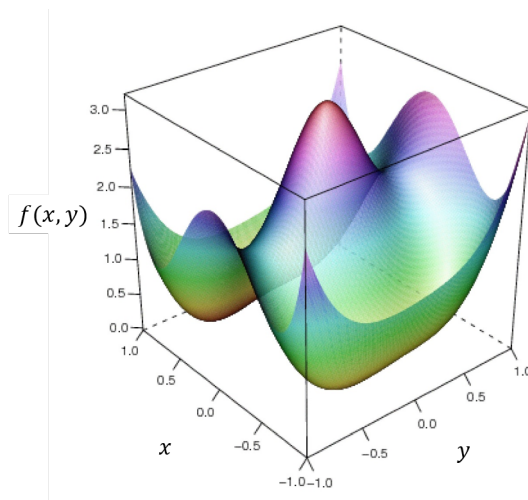


Figure 3: Illustration of the deterministic function f .

We consider two steps for studying this test function. First, the validation criteria are used to compare the results obtained by using different covariance functions in order to identify the most appropriate one for the dataset (as done in Demay et al. (2022)).

Then, a regular squared grid is considered to sample the input space, composed here of 144 observations. On this dataset, the ordinary kriging model is fitted with different covariance functions, namely three Matérn covariances and the Gaussian covariance with a nugget effect for the latter of 10^{-6} (to improve the numerical stability of the covariance matrix inversion). For each of these covariances, the validation criteria are estimated by a cross validation process. The results are presented in Table 1 for ordinary kriging, in Table 2 for Bayesian kriging and in Figure 4.

| Covariance | Q^2 | PVA | PIA | $MSE\alpha$ |
|------------|-------|-------|-------|-------------|
| Matérn 1/2 | 0.95 | 0.99 | 0.98 | 0.056 |
| Matérn 3/2 | 0.99 | 0.91 | 0.90 | 0.073 |
| Matérn 5/2 | 1.00 | 0.65 | 0.63 | 0.073 |
| Gaussian | 1.00 | 0.05 | 0.07 | 0.011 |

Table 1: Validation criteria for the ordinary kriging with different covariance functions, on the sample of $n = 144$ observations of function f .

| Covariance | Q^2 | PVA | PIA | $MSE\alpha$ |
|------------|-------|-------|-------|-------------|
| Matérn 1/2 | 0.95 | 1.09 | 1.06 | 0.061 |
| Matérn 3/2 | 0.99 | 1.62 | 1.60 | 0.106 |
| Matérn 5/2 | 1.00 | 1.58 | 1.55 | 0.106 |
| Gaussian | 1.00 | 0.13 | 0.16 | 0.002 |

Table 2: Validation criteria for the Bayesian kriging with different covariance functions, on the sample of $n = 144$ observations of function f .

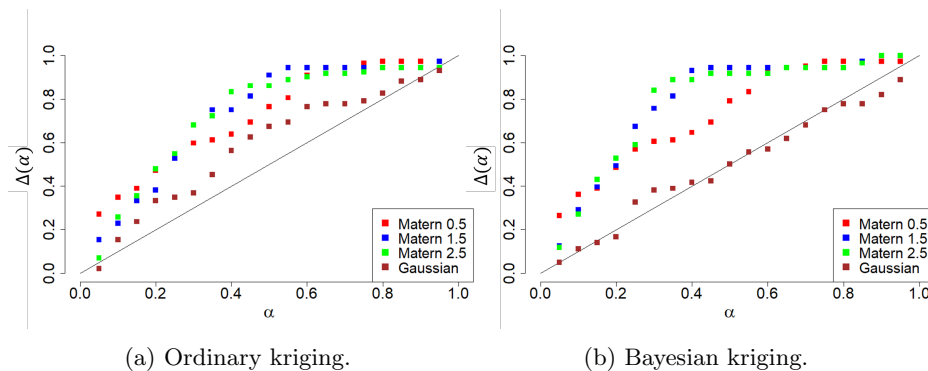


Figure 4: α -CI plots for the ordinary and Bayesian kriging with different covariances functions, on the sample of $n = 144$ observations of function f .

The results show that, in this case, a Gaussian covariance function is the most appropriate covariance function w.r.t. to the different criteria. This result is not

surprising since the test function is smooth and shows large correlations between observations. Although the differences between Q^2 are very small between the Gaussian and Matérn models (except for the Matérn 1/2 model), significant differences appear for the PVA and PIA . These differences become smaller for the $MSE\alpha$. This shows the importance of using simultaneously various criteria for a better assessment of the model performance and accuracy.

Once our covariance model is chosen (the Gaussian one in this case), we can apply a similar test protocol than in Section 4.1. In order to generate datasets, we have to slightly modify the protocol. Since the function is deterministic, choosing a specific geometry for a fixed dataset size will not allow to generate different datasets. Therefore we discard here the regular grid and choose to sample random positions in the input space. The observed dispersion in the results of this section is affected by that choice. This sampling is repeated 100 times for each data set sizes, up to 150 observations.

The results are presented in Figure 5. The values of the Q^2 criterion lead to the same conclusions as for the data from Gaussian process trajectories, in the previous section. We again find better performance with Bayesian kriging, especially for small sample sizes. Note that we have higher Q^2 's than for the previous test case due to the high regularity of the function f .

Significant differences arise with the PVA , PIA and $MSE\alpha$ criteria. Indeed, these criteria do not decrease steadily and monotonically with the number of observations. Moreover, they behave differently depending on the type of kriging. More precisely, for Bayesian kriging, the PVA , PIA and $MSE\alpha$ increase between 20 observations and 50 observations, before decreasing, whereas they keep increasing for ordinary kriging. For datasets made of 50 observations or less, Bayesian kriging seems to under-perform when compared to ordinary kriging but outperform ordinary kriging for more than 50 observations. Still, once the size of the datasets exceed 80 observations, we observe similar results to those obtained with the simulated datasets.

To explain these results, we recall that the initial assumption whereby the function f is a trajectory of a Gaussian process is not verified here, at least for datasets of 50 or less observations. It is therefore possible to obtain poorer criteria as the dataset size increases. We still get good prediction accuracy, since the median of the Q^2 criterion stays between 0.7 and 1 for all dataset sizes and kriging methods, but the predicted variances do not seem to be very accurate, yielding poorly estimated confidence and credible intervals. We can observe that once the dataset size exceeds 80 observations, the evolution of the validation criteria shows that the initial assumption is now valid.

In conclusion, in this deterministic function case for which the initial assumption of a random field is not ensured, Bayesian kriging seems to be more robust than ordinary kriging. Caution is still advised, since in some cases ordinary kriging seems to perform better than Bayesian kriging, as illustrated with the $n = 40$ or $n = 50$ observations' dataset.

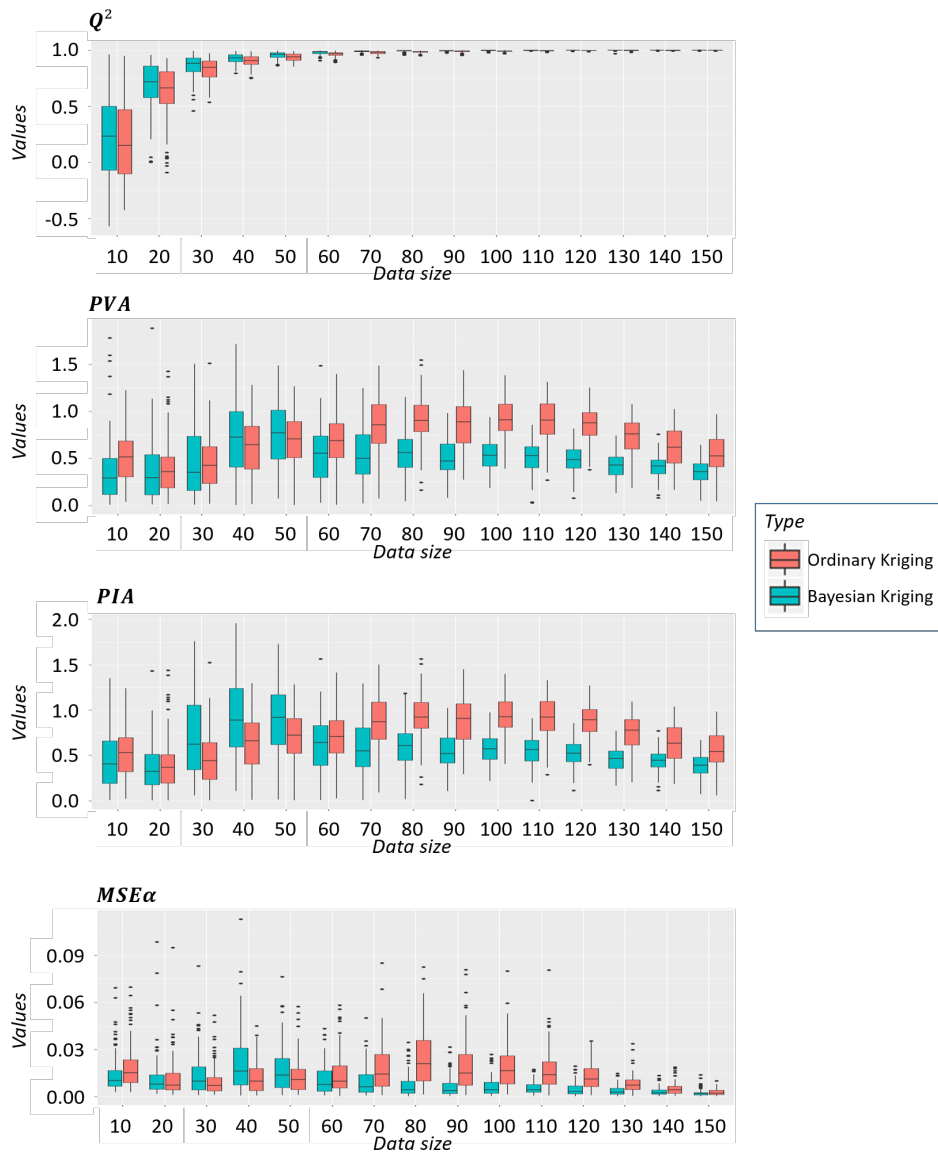


Figure 5: Distribution of validation criteria (Q^2 , PVA, PIA, and MSE_α) w.r.t. the size of datasets, for the deterministic function f .

5 Real application case: G3's dataset

This dataset is made of 70 observations of radioactivity measurements coming decommissioning project of the CEA Marcoule G3 reactor (CEA 2009). They

are sampled in the input domain $[0, 10] \times [0, 7]$. The dataset is mapped in Figure 6. A first kriging modeling using the full dataset is given by Figure 7. More precisely, the prediction maps obtained with ordinary and Bayesian kriging with an exponential covariance for both are given. These prediction maps show small apparent differences between both methods, since the number of observations is high. Let us now see if the same is true if we reduce the sample size and vary the covariance.

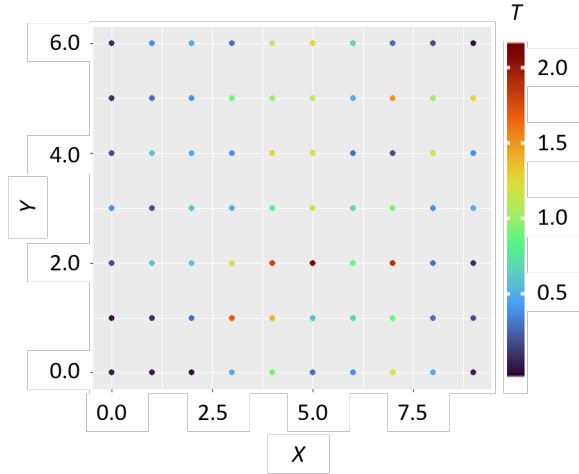


Figure 6: Mapping of G3 observations

Then, a similar test protocol as in Section 4 is applied to assess the behaviour of kriging models according to n . First, let us consider ordinary kriging for different covariance functions, applied to the initial set of 70 observations. The validation criteria estimated by cross-validation are given in Table 3 and Figure 8. For Bayesian kriging, they are given in Table 4 and Figure 8. The results indicate that the Matérn 1/2 model is the best choice in regards of our different criteria since it maximizes the Q^2 criterion while minimizing both PVA and PIA criteria (it also performs well for the $MSE\alpha$ criterion, while not being the function minimizing it overall). Therefore only the Matérn 1/2 covariance function is considered.

To generate multiple datasets, we resample without replacement datasets of various sizes $n = 20, 30, 40, 50, 60, 70$, with the last one being the original dataset. Once again, the process is repeated 100 times for each sample size (except for 70 observations) and for each sample a cross-validation is applied to estimate the validation criteria.

The obtained results are summarised in Figure 9. For the Q^2 criterion, the median values increase from about 0 ($n = 10$) to 0.38 ($n = 70$) for both kriging methods. Slightly higher results are obtained for Bayesian kriging, especially for small sample sizes. The dispersion of Q^2 is similar between the two kriging

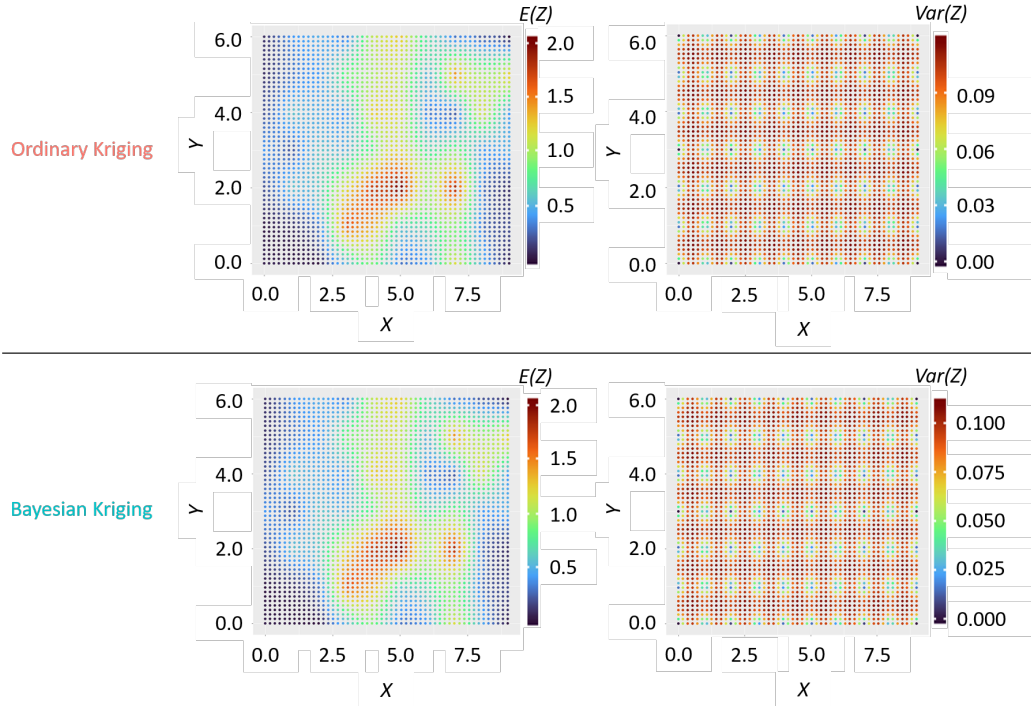


Figure 7: Mapping of predictions obtained with ordinary (top) and Bayesian (bottom) kriging. Kriging predictor (left) and predictive variance (right) are plotted.

| Covariance | Q^2 | PVA | PIA | $MSE\alpha$ |
|--------------------------|-------|-------|-------|-------------|
| Matérn 1/2 (exponential) | 0.37 | 0.06 | 0.07 | 0.0015 |
| Matérn 3/2 | 0.33 | 0.12 | 0.14 | 0.0010 |
| Matérn 5/2 | 0.31 | 0.14 | 0.15 | 0.0014 |
| Gaussian | 0.24 | 0.16 | 0.18 | 0.0021 |

Table 3: Validation criteria for the ordinary kriging with different covariance functions, on the G3 sample of $n = 70$ observations.

methods. The obtained Q^2 estimates here are very low, which normally means that the model is not predictive enough. As our objective is only to compare the kriging methods, this problem is not further investigated here.

Regarding now the PVA , the median values decrease from 0.47 to 0.16 for ordinary kriging, compared to much lower values for Bayesian kriging, namely from 0.19 to 0.06. For the PIA , the values are very close to the ones of PVA . For the $MSE\alpha$, the median values go from 0.011 to 0.0017 for the ordinary kriging,

| Covariance | Q^2 | PVA | PIA | $MSE\alpha$ |
|--------------------------|-------|-------|-------|-------------|
| Matérn 1/2 (exponential) | 0.38 | 0.12 | 0.07 | 0.0013 |
| Matérn 3/2 | 0.20 | 0.51 | 0.55 | 0.0028 |
| Matérn 5/2 | 0.16 | 1.19 | 1.25 | 0.0284 |
| Gaussian | 0.15 | 0.36 | 0.40 | 0.0015 |

Table 4: Validation criteria for the Bayesian kriging with different covariance functions, on the G3 sample of $n = 70$ observations.

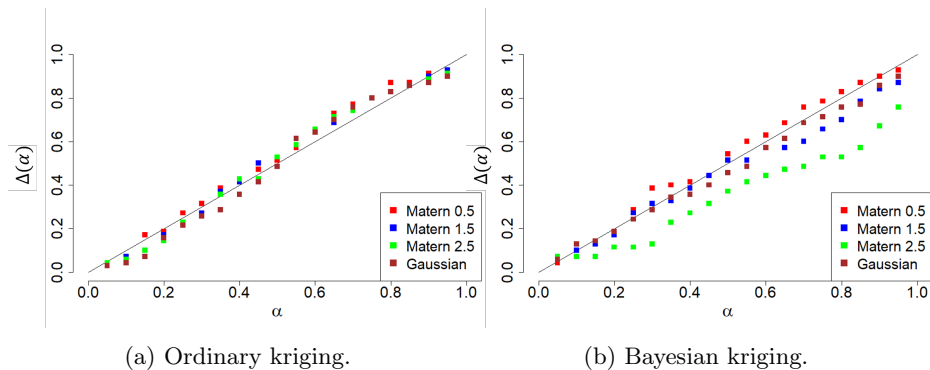


Figure 8: α -CI plots for the ordinary and Bayesian kriging with different covariance functions, on the G3 sample of $n = 70$ observations.

against 0.008 down to 0.0017 for Bayesian kriging. Once again, Bayesian kriging yields better results, especially for smaller datasets. The results of both methods then become almost identical for data sets of 40 or more observations. This is especially visible for the $MSE\alpha$.

We can also remark that the variance of each validation criterion is reduced as the datasets size grows. This is both explained by the larger datasets, but also by our protocol, since observations are randomly drawn without replacement among the original 70 observations. As a result, the samples differ less and less as the dataset sizes increases.

6 Discussion and Conclusions

In conclusion, the use of Bayesian kriging for spatial interpolation of datasets in support of decommissioning and dismantling projects shows promising results. It allows to take into account the uncertainty on the parameters of the kriging model. It is particularly relevant for small datasets for which it outperforms the ordinary kriging in terms of accuracy of predictive mean, variance and predictive intervals. This advantage becomes less important as the sample size increases: ordinary kriging, less computationally expensive, is then preferable for large datasets. Bayesian kriging has also the drawback of requiring a prior specifica-

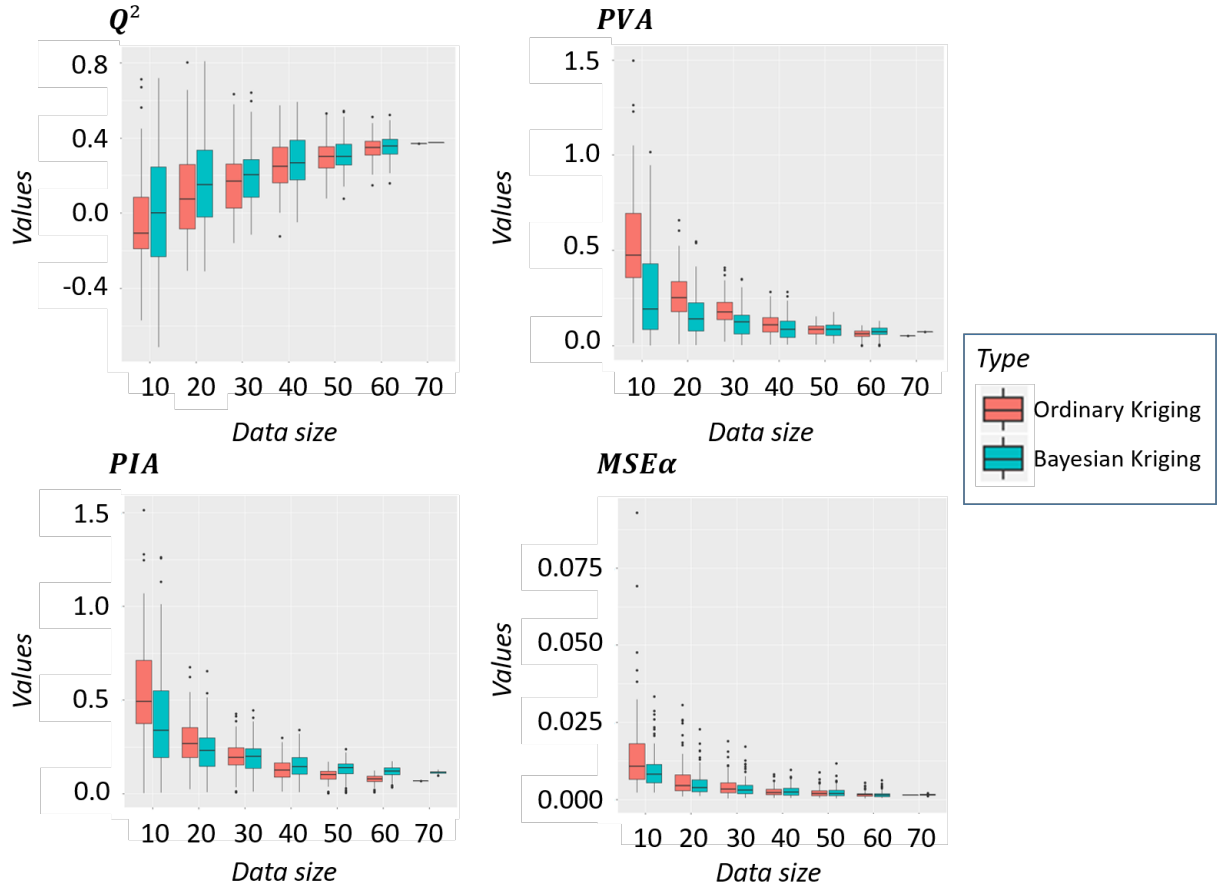


Figure 9: Distribution of validation criteria (Q^2 , PVA , PIA , and MSE_α) w.r.t. the size of datasets, for the G3 dataset.

tion, which is often difficult to choose and can strongly influence the predictions. Therefore, the use of Bayesian kriging should be restricted to smaller datasets or cases in which prior information on parameters is well known.

In our work we did not use the nugget effect as a modelling tool but only as a regularisation of the Gaussian covariance function. Future works will aim at adding this parameter in the model. This could be taken further by considering a heteroscedastic model (Ng and Yin 2012), since the usual nugget effect is formulated as a homoscedastic model. This could be extremely useful and show promising results in the framework of D&D of nuclear sites since radioactive measurements are prone to varying measurement uncertainties, depending on the measuring technique.

7 Appendix: sensitivity analysis to the prior distribution of parameters

The choice of prior specifications is a complicated step in Bayesian analysis. We therefore conduct a sensitivity analysis to justify our use of an improper prior on the mean and variance parameters. Note that the range will not be described here, since no usual specification is available.

First, it could be argued that the prior on the parameter β is chosen improper since this choice is implicitly made in ordinary kriging:

$$\pi(\beta) \propto 1.$$

Second, for the variance parameter σ^2 , several choices for priors can be considered. To give a quick overview of our test protocol, we used a simulated dataset, defined as random trajectories of the same Gaussian process model as in Section 4.1. An initial dataset of 16641 observations is simulated, on which the parameters β_{init} and σ_{init}^2 are estimated. These estimations will be considered as reference values for our prior specifications. From these 16641 observations, samples of $n = 20$ and $n = 50$ observations are randomly drawn. This sampling is then repeated 100 times, generating a total of 200 datasets. Then, for each dataset, the Bayesian kriging is applied considering five different prior specifications:

1. vague with

$$\pi(\beta, \sigma^2) \propto \frac{1}{\sigma^2},$$

2. correctly centred and informative with

$$\sigma^2 \sim \text{Scaled-Inv-}\chi^2(\sigma_{\text{init}}^2, n) \text{ and } \beta|\sigma^2 \sim \mathcal{N}(\beta_{\text{init}}, \frac{\sigma^2}{n}),$$

3. incorrectly centred and informative with

$$\sigma^2 \sim \text{Scaled-Inv-}\chi^2(3\sigma_{\text{init}}^2, n) \text{ and } \beta|\sigma^2 \sim \mathcal{N}(3\beta_{\text{init}}, \frac{\sigma^2}{n}),$$

4. correctly centred and non-informative with

$$\sigma^2 \sim \text{Scaled-Inv-}\chi^2(\sigma_{\text{init}}^2, \frac{n}{3}) \text{ and } \beta|\sigma^2 \sim \mathcal{N}(\beta_{\text{init}}, \frac{\sigma^2}{n}),$$

5. incorrectly centred and non-informative with

$$\sigma^2 \sim \text{Scaled-Inv-}\chi^2(3\sigma_{\text{init}}^2, \frac{n}{3}) \text{ and } \beta|\sigma^2 \sim \mathcal{N}(3\beta_{\text{init}}, \frac{\sigma^2}{n}).$$

For each prior specification, validation criteria are estimated by cross-validation. The obtained results are given in Figure 10. First, we observe that the Q^2 criterion is not sensitive to the prior specification. This is expected since the prediction performances depend mostly on the number of observations and on the geometry of the dataset. On contrary, the PVA and PIA criterion are very sensitive to the prior specification since prediction variance highly depends on parameter estimation. A vague prior allows to mitigate the bias introduced with an incorrectly centred prior, as case 3 shows a worse result than case 5. We can also see that even with a correctly centred and informative prior (case 2), the gains in parameter estimation are small if we compare it to a vague specification (case 1).

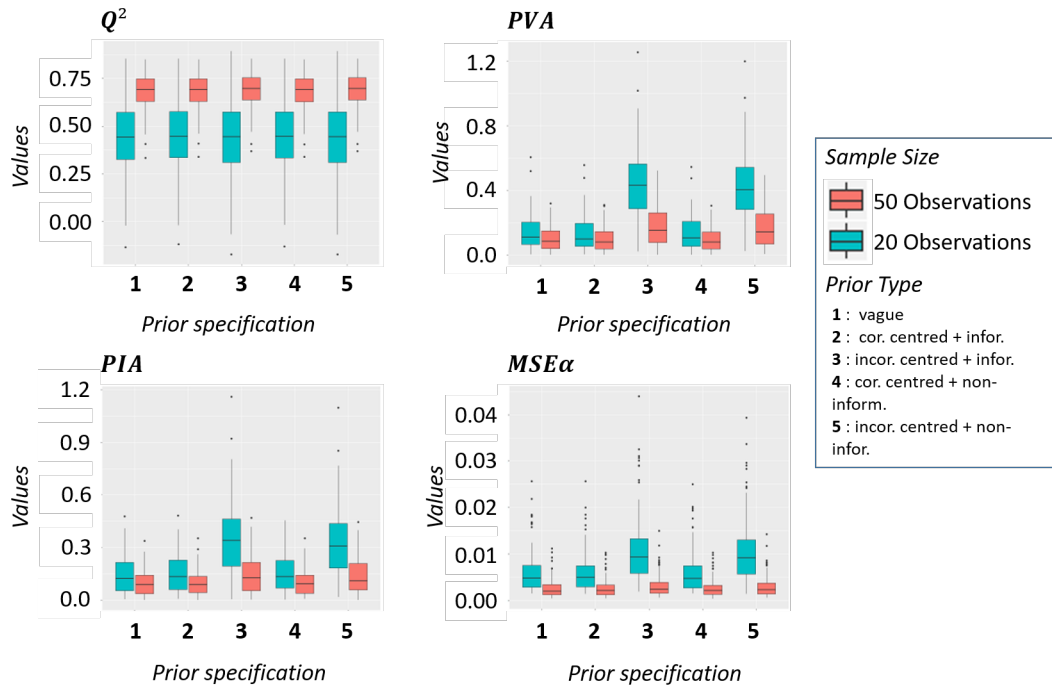


Figure 10: Distribution of validation criteria (Q^2 , PVA , PIA , and $MSE\alpha$) w.r.t. to the prior specification.

In conclusion, the choice of a vague or improper prior seems to be reasonable, as the improvements provided by a correctly specified prior do not seem good enough in comparison to the pitfall of a bad prior specification. These results are also similar to the one obtained by Helbert et al. (2009).

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