Conservative estimates of excursion sets in reliability engineering

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Résumé. Dans le cadre de la modélisation par processus Gaussiens, nous nous penchons sur un problème d'estimation d'ensemble d'excursion pour une fonction chère à évaluer. L'espérance de Vorob'ev, récemment revisitée dans ce contexte, donne une estimation de l'ensemble d'excursion sous une contrainte de volume égal au volume d'excursion moyen, mais ne permet pas directement de tirer des conclusions en termes d'ensemble de confiance. L'espérance de Vorob'ev est en effet un ensemble de niveau particulier de la probabilité de couverture, c'est à dire d'une probabilité marginale de dépassement de seuil pour le champ Gaussien sous-jacent. Il a été montré récemment en se concentrant plus spécifiquement sur les probabilités jointes d'excursion en plusieurs points qu'il était possible de construire des ensembles de confiance dans le cas des champs Gaussiens Markoviens. De tels ensembles de confiance sont définis comme ensembles de volume maximal parmi les ensembles de probabilité donnée d'être contenu dans l'ensemble d'excursion. Nous étendons ici cette approche au cas non-Markovien et explorons plusieurs pistes pour améliorer le calcul de la probabilité jointe d'excursion en plusieurs points. De plus, nous appliquons cette méthode pour obtenir une estimation conservative de l'ensemble des configurations sûres dans le cadre d'un cas test IRSN en sûreté-criticité nucléaire. Nous introduisons finalement une stratégie de réduction d'incertitude pour l'estimation conservative séquentielle d'un ensemble d'excursion.

Mots-clés. Problèmes inverses, Méthodes bayésiennes, Plan dexpérience, Études de cas

Abstract. In the framework of Gaussian random field modeling, we focus on the problem of estimating the excursion set of a function under a limited evaluation budget. The recently revisited Vorob'ev expectation gives a practical estimate with the property of preserving the expected volume of excursion, however it is not directly possible to provide interpretations in terms of confidence regions. The Vorob'ev expectation is, in fact, a specific level set of the coverage probability function, the marginal probability of excursion of the underlying posterior Gaussian field. By shifting the focus on the joint probability of excursion it was recently shown that it is possible to compute a joint confidence statement on the estimate of the excursion set in the case of a Gauss Markov random field. This estimate is computed as the largest set among the ones that have probability at least α of being inside the excursion set. Here we extend this approach to the non-Markovian case and we investigate different ways to improve the approximation of the joint probability of excursion. Moreover we apply this method to provide conservative estimates of safe configurations for a nuclear criticality safety test case. Finally we introduce an uncertainty reduction strategy for sequentially learning conservative estimates.

Keywords. Inverse problems, Bayesian methods, Experimental design, Case studies

1 Introduction

In this work we present a set estimation approach for inversion problems of an expensive to evaluate objective function. In particular we are interested in estimating the set of configurations where a given response is above a certain threshold.

We consider a continuous objective function $f : D \subset \mathbb{R}^d \to \mathbb{R}$ and, given a prescribed threshold $T \in \mathbb{R}$, we are interested in the excursion set

$$\Gamma^\star = f^{-1}([T, +\infty)) = \{x \in D : f(x) \geq T\}.$$

In reliability engineering, the set $\Gamma^\star$ often represents the set of unsafe configurations of a system depending on d parameters. For example, in the test case provided by the department of nuclear criticality safety of the French Institute of Nuclear Safety which is presented in the following section, the set of unsafe configurations is represented by the excursion set of the function $k_{\text{effective}}$ above the level $T = 1$.

Following the Gaussian random field (GRF) modeling approach (see e.g. [6]), the function f is considered as a realization of $Z = (Z_x)_{x \in D}$, a GRF with continuous sample paths whose mean function and covariance kernel are denoted with m and k respectively. The excursion set $\Gamma^\star$ is then regarded as a realization of the random closed set

$$\Gamma = \{x \in D : Z_x \geq T\}.$$

We assume that the function has been evaluated at few points $\mathbf{X}_n = \{x_1, \ldots, x_n\}$ and we consider the posterior field $(Z_x)_{x \in D} \mid \mathcal{A}_n$ where $\mathcal{A}_n := (Z_{x_1} = f(x_1), \ldots, Z_{x_n} = f(x_n))$. We denote with m_n and k_n the posterior mean function and covariance kernel respectively.

The field $(Z_x)_{x \in D} \mid \mathcal{A}_n$ defines a posterior distribution for the random closed set $\Gamma \mid \mathcal{A}_n$. In the theory of random closed sets several definitions of expectation are available to summarize this distribution (see e.g. [5]), in particular in [2] the Vorob'ev expectation was revisited in the framework of set estimation and uncertainty quantification under Gaussian random field priors. This expectation relies on the coverage probability function

$$p_n : x \in D \to p_n(x) = P_n(x \in \Gamma) := P(x \in \Gamma \mid \mathcal{A}_n) \in [0, 1]$$

which gives the point-wise probability of excursion. As Z is a Gaussian field, the coverage probability function can be computed analytically as $p_n(x) = P_n(Z_x \geq T) = \Phi\left(\frac{m_n(x)-T}{k_n(x,x)}\right)$.

The level sets of p_n naturally define quantiles of $\Gamma \mid \mathcal{A}_n$, called Vorob'ev quantiles, $Q_\rho = \{x : p_n(x) \geq \rho\}$. The Vorob'ev expectation is the specific level set Q_{ρ^*} such that $|Q_{\rho^*}| = \mathbb{E}[|\Gamma|]$, where $|\cdot|$ is the Lebesgue measure of the set.

The Vorob'ev quantiles involve marginal confidence statements on the probability of excursion, thus they do not provide a joint confidence statement on the probability of observing a specific set. In particular it is not possible to obtain a set where with probability α the response exceeds the threshold at each of its locations.

2 Conservative estimates

In order to obtain a joint type of confidence statements the concept of *conservative estimates* was recently introduced in [1], that is a set

$$E_{T,\alpha} \in \arg\max_E \{|E| : P_n(E \subset \{Z_x \geq T\}) \geq \alpha\}.$$

In general the set of maximum volume is not unique however, in practice, the optimization is conducted over parametric families and a unique optimum is reached. In this work we restrict the optimization to a one dimensional parametric family for E, hence in the following, with an abuse of notation, we denote with $E_{T,\alpha}$ the set that realizes the maximum. With such a remark in mind then, $E_{T,\alpha}$ is the largest set where, with probability α, the threshold T is exceeded at each of its locations.

In reliability engineering $E_{T,\alpha}$ is the set that with probability α consists of only configurations where the response is above a certain level, which are often dangerous configurations. Frequently however the engineers are interested in the set that, with probability α, contains all potentially dangerous zones to avoid or, reciprocally, in the set that, with probability α, contains only safe configurations. Those sets can be formalized as the conservative estimate for the lower excursion and the credible regions.

We define conservative estimate for the lower excursion the set

$$E^-_{T,\alpha} = \arg\max_E \{|E| : P_n(E \subset \{Z_x < T\}) \geq \alpha\}.$$

$E^-_{T,\alpha}$ is the largest set such that, with probability α, the response is below the threshold T at each of its locations.

A closely related concept is the set of credible regions, the complement of $E^-_{T,\alpha}$

$$C_{T,\alpha} = (E^-_{T,\alpha})^C = \left(\arg\max_E \{|E| : P_n(E \subset \{Z_x < T\}) \geq \alpha\}\right)^C.$$

This is the set that contains, with probability α, all possible excursions greater or equal to T.

The estimate of $P_n(E \subset \{Z_x \geq T\})$ is obtained by relying on a fast Monte Carlo algorithm to approximate a truncated multivariate normal which generalizes the algorithm introduced in [1].

The maximization of the volume is computed over the parametric family of Vorob'ev quantiles. While this family presents nice properties, notably it is a family of nested sets, further families could be explored to obtain a better approximation of the set with largest volume.

3 Test case

In this section we present a real-life application that was provided by the department of nuclear criticality safety of the French Institute of Nuclear Safety (IRSN, Institut de Radioprotection et de Sûreté Nucléaire).

The safety of a fissile material storage facility is measured with the neutron multiplication factor $k_{\text{effective}}$. A value of $k_{\text{effective}} \geq 1$ denotes an increasing neutron production, thus an unsafe configuration, while $k_{\text{effective}} < 1$ denotes a safe configuration. In the present case study we consider the safety of a storage facility containing cylinders of fissile material of diameter l with total mass m_{tot}. The function $k_{\text{effective}}$ for this type of configurations is modeled as

$$k_{\text{effective}} : (l, m_{tot}) \in \mathbb{R}^2 \longrightarrow \mathbb{R}.$$

The parameters are expressed in cm and g respectively and they are constrained into the intervals $l \in [7.8, 24], m_{tot} \in [350, 35000]$. Here both variables are rescaled to the unit interval $[0, 1]$. The excursion set of interest is

$$\Gamma^\star = \{\mathbf{x} = (l, m_{tot}) \in [0,1]^2 : k_{\text{effective}}(l, m_{tot}) < 1\}.$$

Figure 1 shows a benchmark estimate of the excursion set obtained by evaluating the function on a grid, the region of interest is plotted in white.

In the setting previously introduced we define a prior GRF Z with unknown constant mean function and a tensor product Matérn ($\nu = 5/2$) kernel; from 15 observations $(\mathbf{x}_i, k_{\text{effective}}(\mathbf{x}_i))_{i=1,\dots,15}$ we estimate the parameters of the model by Maximum Likelihood and we compute the posterior GRF $Z \mid (Z_{\mathbf{x}_i} = k_{\text{effective}}(\mathbf{x}_i))_{i=1,\dots,15}$. The excursion $\Gamma^\star$ can be regarded as a realization of the random closed set $\Gamma \mid (Z_{\mathbf{x}_i} = k_{\text{effective}}(\mathbf{x}_i))_{i=1,\dots,15}$ and the Vorob'ev expectation is an estimator for $\Gamma^\star$. Here, however, we are interested in a robust estimate of $\Gamma^\star$ so we consider the conservative estimate $E^-_{T=1,\alpha=0.95}$. Figure 2 shows the conservative estimate of the safe regions compared with the contour line of the true excursion region and with the countour line of the Vorob'ev quantile at 95%.

Several approximations are involved in the computation of the conservative estimates: the GRF assumption, the chosen model and the covariance parameters estimation. The

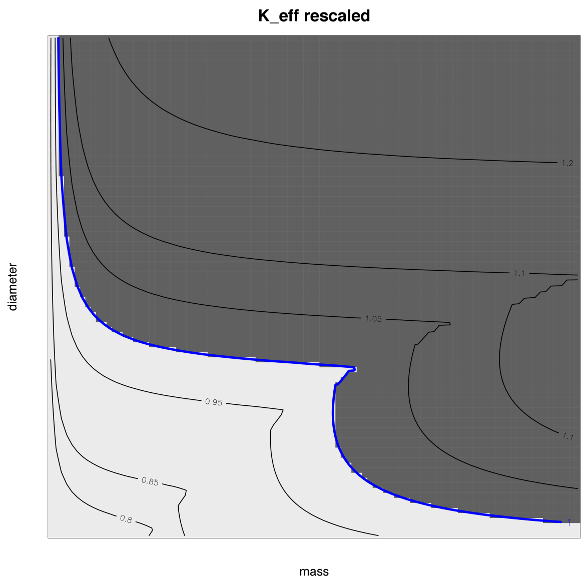

Figure 1: $k_{\text{effective}}$ evaluated on a regular grid on $[0,1]^2$. In blue the contour line $k_{\text{effective}} = 1$, the true safe region is the light gray area.

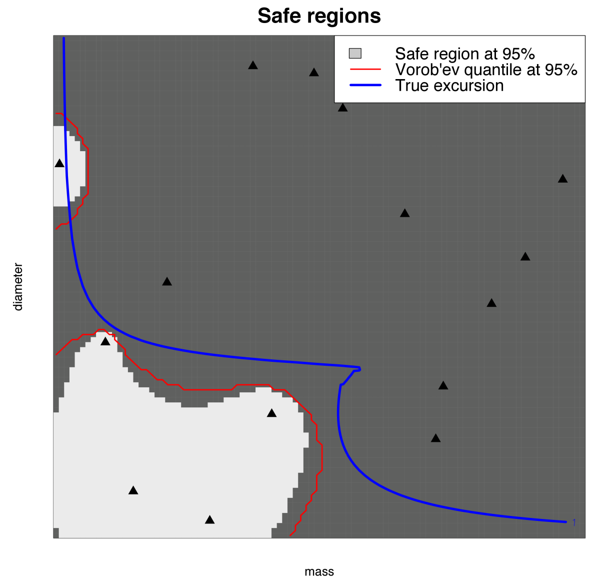

Figure 2: Safe region estimate at 95% (clear region) based on evaluations of $k_{\text{effective}}$ at 15 locations (black triangles) compared with Vorob'ev quantile at 95% (red line)

conservative estimate approach is intrinsically safer than the Vorob'ev expectation approach because it considers the joint probability of excursion, however the approximations mentioned above still affect the estimate. Those effects could be mitigated with a worst case/full Bayesian approach on the model parameters or also with sequential design strategies to adaptively reduce both model and set estimation uncertainties. In our talk we focus on the latter point.

4 Sequential uncertainty reduction strategies for conservative estimates

The uncertainty associated with GRF models has been measured and used with favorable outcomes in the design and analysis of computer experiments [7] and in global optimization [4]. Recently (see e.g. [3] and references therein) this measure has been used in inversion problems, in particular fast Stepwise Uncertainty Reduction (SUR) strategies have been implemented for the problem of estimating excursion regions. A SUR strategy aims at constructing a sequence of evaluation points of f such that the uncertainty on a given quantity of interest is reduced. In [3] (section 4.2) a SUR strategy for reducing the uncertainty on the excursion set estimate was defined with the uncertainty function

$\mathcal{H}_n(\mathcal{A}_n) = \mathrm{Var}_n(\Gamma) = \mathbb{E}\left(|\Gamma \Delta Q_{\rho^*}| \mid \mathcal{A}_n\right)$, where Q_{ρ^*} is the Vorob'ev expectation of $\Gamma \mid \mathcal{A}_n$, $A \Delta B$ denotes the symmetric difference between the sets A, B and $|\cdot|$ is the Lebesgue measure of the set. Here we adapt this SUR strategy to conservative estimates and we propose a new ad hoc heuristic strategy.

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