

Supplementary material for Adaptive Design of Experiments for Conservative Estimation of Excursion Sets.

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A Complements on conservative estimates

The following result here presented as a corollary of Proposition 1, is a well known result Molchanov (2005) for the Vorob'ev expectation.

Corollary 1 (of Proposition 1). The Vorob'ev expectation Q_{ρ_V} minimizes the expected distance in measure with Γ among all measurable (deterministic) sets M such that $\mu(M) = \mu(Q_{\rho_V})$. Moreover if $\rho_V \geq \frac{1}{2}$, then the Vorob'ev expectation also minimizes the expected distance in measure with Γ among all measurable sets M that satisfy $\mu(M) = \mathbb{E}[\mu(\Gamma)]$.

Proof of Corollary 1. The first statement is a direct application of Proposition 1 with $\rho = \rho_V$.

For the second statement, by definition we have that either $\mu(Q_{\rho_V}) = \mathbb{E}[\mu(\Gamma)]$ or $\mu(Q_\rho) < \mathbb{E}[\mu(\Gamma)] \leq \mu(Q_{\rho_V})$ for each $\rho > \rho_V$. In the first case we can directly apply Proposition 1. In the second case we can apply the same reasoning as in the proof of Proposition 1 however in last step of the proof we need to impose $\rho_V \geq \frac{1}{2}$ for obtaining the result. □

In general, the Vorob'ev quantile chosen for CE_α is not the set S with the largest measure μ that has the property $P(S \subset \Gamma) \geq \alpha$ as shown in the counterexample below.

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Example 1. Consider a discrete set $D = \{x_1, x_2, x_3, x_4\}$, a random field $(Z_x)_{x \in D}$ and assume that $\Gamma = \{x \in D : Z_x \geq 0\}$. In this framework we show the existence of a conservative set at level $\alpha = 0.5$ larger than the largest Vorob'ev quantile with the same conservative property.

Assume that for some $\rho_1 \in [0, 1]$

$$P(Q_{\rho_1} \subset \Gamma) = P(Z_{x_1} \geq 0, Z_{x_2} \geq 0) = 1/2,$$

where $Q_{\rho_1} = \{x_1, x_2\}$ is a Vorob'ev quantile at level ρ_1 , that is $P(Z_{x_1} \geq 0), P(Z_{x_2} \geq 0) \geq \rho_1$.

Note that in the case where $Z_{x_1} \perp\!\!\!\perp Z_{x_2}$, the Vorob'ev level is automatically determined as $\rho_1 = \sqrt{2}/2$ and if $Z_{x_1} = Z_{x_2}$ a.s., then $\rho_1 = 1/2$. Let us assume here that $Z_{x_1} \neq Z_{x_2}$, which implies $\rho_1 \in (1/2, \sqrt{2}/2)$. Let us further denote with Ω_1 the subset of Ω such that for all $\omega \in \Omega_1$ $\min(Z_{x_1}(\omega), Z_{x_2}(\omega)) \geq 0$ and define $\Omega_2 = \Omega \setminus \Omega_1$.

We further fix the random variable Z_{x_3} as

$$Z_{x_3}(\omega) = \begin{cases} 1 & \text{if } \omega \in \Omega_1 \\ -1 & \text{if } \omega \in \Omega_2. \end{cases}$$

Then $P(Z_{x_3} \geq 0) = P(\min(Z_{x_1}, Z_{x_2}) \geq 0) = P(Z_{x_1} \geq 0, Z_{x_2} \geq 0) = 1/2$. Moreover $P(\min(Z_{x_1}, Z_{x_2}, Z_{x_3}) \geq 0) = 1/2$, i.e. $\{x_1, x_2, x_3\}$ has the conservative property at level $\alpha = 0.5$.

Consider $\Omega_3 \subset \Omega_1$ with $P(\Omega_3) = 1/3$ and $\Omega_4 \subset \Omega_2$ with $P(\Omega_4) = 1/3$. Define

$$Z_{x_4}(\omega) = \begin{cases} 1 & \text{if } \omega \in \Omega_3 \cup \Omega_4 \\ -1 & \text{otherwise.} \end{cases}$$

We now have that $P(\min(Z_{x_1}, Z_{x_2}, Z_{x_3}, Z_{x_4}) \geq 0) = 1/3 < 1/2$ and $P(Z_{x_4} \geq 0) = 1/3 + 1/3 > 1/2$. Under this construction the Vorob'ev quantiles are $Q_{\rho_1} = \{x_1, x_2\}$, $Q_{\rho_2} = \{x_1, x_2, x_4\}$ and $Q_{0.5} = D$. The set $\{x_1, x_2, x_3\}$ is therefore the conservative set at level $\alpha = 0.5$, as it is the largest subset of D with the conservative property, however it is not a Vorob'ev quantile.

B Sequential conservative excursion set estimation: procedure overview

Consider a function $f : \mathbb{X} \rightarrow \mathbb{R}$, we are interested in estimating

$$\Gamma^* = \{x \in \mathbb{X} : f(x) \geq t\}, \quad t \in \mathbb{R}.$$

from few evaluations. We consider a prior Gaussian process $(Z_x)_{x \in \mathbb{X}}$ with prior mean \mathbf{m} and covariance kernel \mathfrak{K} . The estimation procedure often starts with a small initial design \mathbf{X}_n , $n \geq 1$, where n is often chosen as a function of the input space dimension. If $\mathbb{X} = \mathbb{R}^d$, as a rule of thumbs, the initial number of evaluations is often $n = 10d$. In our framework, often, the initial design is

chosen as space filling, such as a Latin hypercube sample (LHS) design or points from a low discrepancy sequence such as the Halton and the Sobol' sequence. In Algorithm 1 we summarize the main steps for computing conservative estimates and evaluating their uncertainties.

Algorithm 1: Sequential conservative excursion set estimation.

Input : N_{tot} maximum number of evaluations, n size of initial design, q size of batches, function f , threshold t , criterion J , uncertainty function H

Output: $Q_{N_{tot}, \rho_{N_{tot}}^\alpha}$ for Γ^* and the uncertainty value H_N

initial DoE select initial DoE \mathbf{X}_n , e.g., with space filling design;
 evaluate the function f at \mathbf{X}_n ;
 compute the posterior model $Z | \mathcal{A}_n$ and the estimate Q_{n, ρ_n^α} ;
 $i = n_0$;

while i less than N_{tot} **do**

update the model $i = i + q$;
 select $\mathbf{x}^{(q)}$ by minimizing $J_i(x)$;
 evaluate the function f at $\mathbf{x}^{(q)}$;
 update the posterior model $Z | \mathcal{A}_i$;
 compute the conservative estimate Q_{i, ρ_i^α} ;

post-processing evaluate the uncertainty function H_i on Q_{i, ρ_i^α} ;

end
 optional post-processing on $Q_{N_{tot}, \rho_{N_{tot}}^\alpha}$;

C Additional numerical results

C.1 Benchmark study on Gaussian processes

In this section we present more details about the test cases on Gaussian process realizations described in Section 5.1.

C.1.1 Dimension 2

Figure 1 shows the type I error for each strategy in Table 1. Strategies B , C and E show a lower type I error with respect to the other strategies, however the all strategies present very low type I error compared to the total expected volume of the set.

Figure 2 shows the total time required to evaluate the criteria and to compute at each step the conservative estimate. The computational time is mainly driven by the size of the conservative estimate. In fact, for conservative estimates with large volumes, the othant probabilities involved in its computation are higher dimensional.

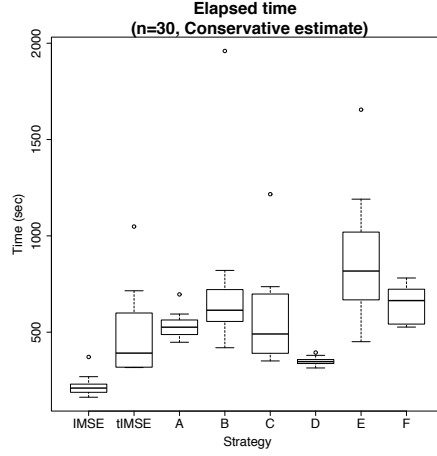
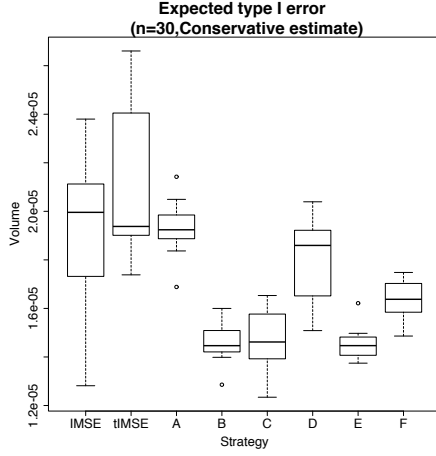


Figure 1: Median type I error for $Q_{\rho_n^\alpha}$, Figure 2: Total time to compute $Q_{\rho_n^\alpha}$, 2-dimensional Gaussian processes test case.

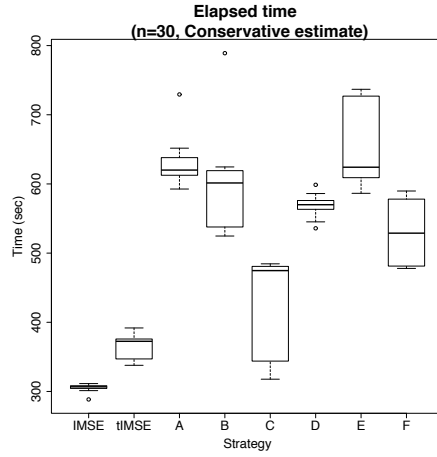
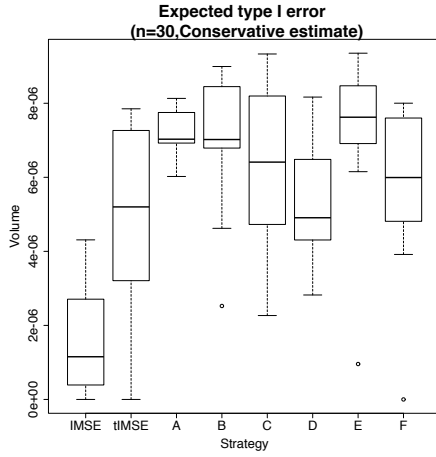


Figure 3: Median type I error for $Q_{\rho_n^\alpha}$, Figure 4: Total time to compute $Q_{\rho_n^\alpha}$, 5-dimensional Gaussian processes test case.

C.1.2 Dimension 5

Figure 3 shows the type I error and Figure 4 shows the total time required to evaluate the criteria and to compute at each step the conservative estimate. In this case strategies IMSE presents a lower type I error. This might be caused by the better global approximation obtained with a model based on a space filling design.

Figure 4 shows the total time required to evaluate the criteria and to compute at each step the conservative estimate.

C.2 Coastal flood test case

In this section we explore the behaviour of the strategies under different scenarios for the covariance hyper-parameters:

1. *fixed initial hyper-parameters (FI)*: the covariance parameters are fixed throughout the sequential procedure as the maximum likelihood estimates obtained from the initial evaluations \mathbf{f}_{10} ;
2. *re-estimated hyper-parameters (RE)*: at each step the hyper-parameter estimates are updated with the new evaluations of the function;

We consider the same experimental setup of Section 5.2, we fix only one initial DoE of $n = 10$ points chosen with the function `lhsDesign` from the package `DiceDesign` (Franco et al., 2013). We run $n = 20$ iterations of each strategy in Table 1 where at each iteration we select one evaluation of f .

Let us start with the case where we estimate the hyper-parameters only using the evaluations of f at \mathbf{X}_{10} . Figures 5, 6 show the type II error and the relative total volume error. These errors are both computed comparing the conservative estimate with the true set obtained with evaluations of f on a fine grid. True type I error, not shown, is equal to zero for each strategy at each iteration. Type II error decreases as a function of the evaluations number for all strategies, in particular strategies B , $tIMSE$, C and E provide a good uncertainty reduction. In particular strategies B , C and E provide a faster uncertainty reduction in the first 10 iterations than the other strategies. Strategy D focuses on reducing the type II error for the Vorob'ev median and it is not well adapted to reduce uncertainties on conservative estimates.

In practice, the covariance parameters are often re-estimated after a new evaluation is added to the model. While this technique should improve the model it leads to better conservative estimates only if the hyper-parameter estimation is stable and reliable. Conservative estimates are in fact based on the coverage probability function and in particular on high quantiles of this function.

Figures 7 and 8 show the Type II and relative volume error computed comparing the conservative estimate to the true set in the case where covariance parameters are re-estimated at each step. During the first 10 iterations, all strategies except IMSE show a small (less than 1%) type I error, not shown, which becomes equal to zero for all strategies after iteration 10.

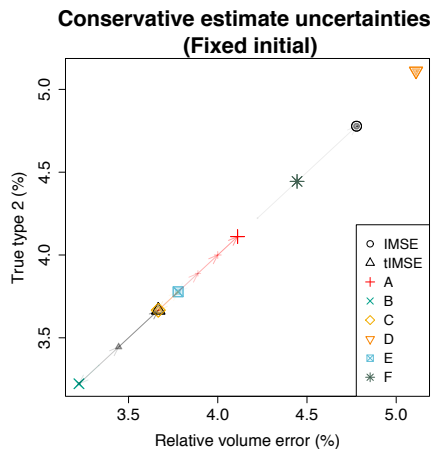


Figure 5: Type II error versus relative volume error for $Q_{\rho_n^\alpha}$ for the last 5 iterations, no re-estimation of the covariance parameters.

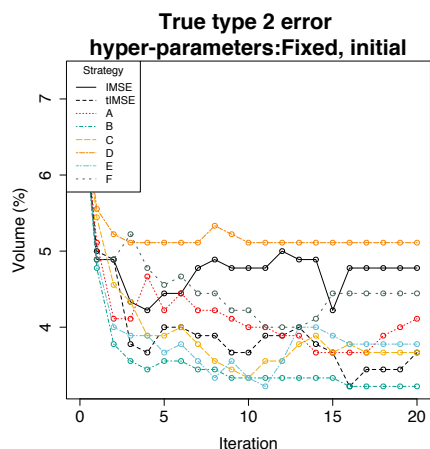


Figure 6: Type II error of $Q_{\rho_n^\alpha}$ at each n computed with respect to the true set, no re-estimation of the covariance parameters.

The strategies IMSE and D still show the worst behaviour among the tested strategies both in terms of true type II error and of relative volume error, however the remaining strategies do not show big differences. The tIMSE show the best behaviour closely followed by Strategy E, C, A . The differences between the final estimated set obtained with these four strategies are small and they are mainly due to a difference in the hyper-parameter estimation. The tIMSE strategy produces more stable hyper-parameter estimators than Strategy E , where the range parameters decrease in the last steps. This change leads to smaller more conservative set estimates.

If the covariance hyper-parameters are kept fixed, Figure 6 shows that the true type II error tends to stabilize because the conservative estimate is the best according to the current model. On the other hand the re-estimation of the parameters leads to a more unstable type II error which also indicates that the underlying model is adapting to the new observations.

The re-estimation of the covariance parameters at each steps might lead to instabilities in the maximum likelihood estimators. In this test case the parameter estimation is very stable, however further studies are required to better understand the behaviour of maximum likelihood estimators under these circumstances.

References

- Franco, J., Dupuy, D., Roustant, O., Damblin, G., and Iooss, B. (2013). *DiceDesign: Designs of Computer Experiments*. R package version 1.3.

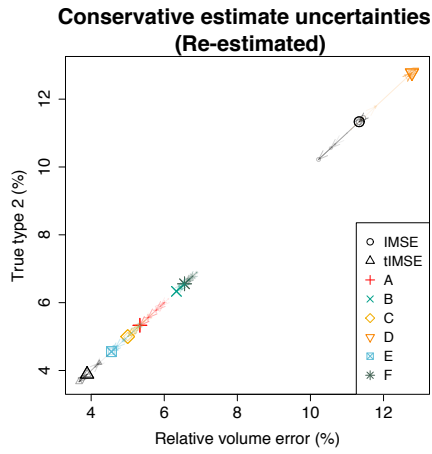


Figure 7: True type II error versus relative volume error for $Q_{\rho_n^\alpha}$ at each n , computed with respect to the true set re-estimation of the covariance parameters at each step.

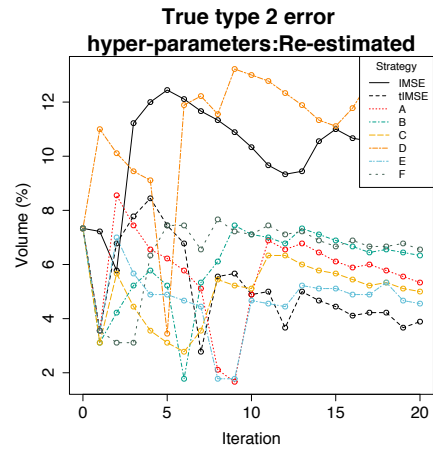


Figure 8: True type II error for $Q_{\rho_n^\alpha}$ at each n , re-estimation of the covariance parameters at each step.

Molchanov, I. (2005). *Theory of Random Sets*. Springer, London.