Bayesian methods for excursion set estimation

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Second workshop on Gaussian Processes at Saint-Étienne: Modèles aléatoires et applications Saint-Étienne, France October 10, 2018

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The framework

In this talk we focus on the problem of determining the set

 $\Gamma^{\star} = \{x \in D : f(x) \in T\} = f^{-1}(T)$

where $D \subset \mathbb{R}^d$ is compact, $f : D \longrightarrow \mathbb{R}^k$ is continuous, $T \subset \mathbb{R}^k$.

Here:
$$k = 1$$
, and $T = (-\infty, t]$ for a fixed $t \in \mathbb{R}$.
 $\Gamma^* = \{x \in D : f(x) \le t\}$ is denoted the excursion set of f below t.

Objective

Estimate Γ^* and quantify uncertainty on it when f is evaluated only at a few points $\mathbf{X}_n = \{x_1, \dots, x_n\} \subset D$.

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Some applications

Moret test case (k_eff)



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Some applications



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Some applications

Coastal flooding



Conclusion

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Selected references

This problem has been tackled in many previous works such as

Sacks, J., Welch, W. J., Mitchell, T. J., and Wynn, H. P. (1989). Design and analysis of computer experiments. Statistical Science, 4(4):409-435.

Ranjan, P., Bingham, D., and Michailidis, G. (2008). Sequential experiment design for contour estimation from complex computer codes. Technometrics, 50(4):527-541.

Bect, J., Ginsbourger, D., Li, L., Picheny, V., and Vazquez, E. (2012). Sequential design of computer experiments for the estimation of a probability of failure. Stat. Comput., 22 (3):773-793.

Chevalier, C., Bect, J., Ginsbourger, D., Vazquez, E., Picheny, V., and Richet, Y. (2014). Fast kriging-based stepwise uncertainty reduction with application to the identification of an excursion set. Technometrics, 56(4):455-465.

Bolin, D. and Lindgren, F. (2015). *Excursion and contour uncertainty regions for latent Gaussian models.* JRSS: B, 77(1):85-106.

among many others



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Main questions tackled in this work

- How to use meta-models, in particular Gaussian processes to estimate the set?
 (Vorob'ev expectation, conservative estimates)
- How to sequentially reduce the uncertainty on such estimates? (SUR strategies for conservative estimates)
- How to visualize the excursion set in high dimensions? (Profile extrema functions)



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The framework: an example



Function $f: D \subset \mathbb{R}^2 \to \mathbb{R}$

- $D = [0,1] \times [0,1]$
- continuous.

Evaluated at n = 15 points $\mathbf{X}_n = (x_1, \dots, x_n)$ (black triangles) with values $\mathbf{f}_n = (f(x_1), \dots, f(x_n))$.

Objective: estimate $\Gamma^* = \{x \in D : f(x) \le t\}$ and evaluate the uncertainty of the estimate.

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Bayesian approach

Bayesian framework: f is seen as one realization of a Gaussian random field (GRF) $(Z_x)_{x \in D}$ with prior mean *m* and covariance kernel *k*.

Given the function evaluations \mathbf{f}_n the posterior field has a Gaussian distribution

$$Z \mid (Z(\mathbf{X}_n) = \mathbf{f}_n)$$

with mean and covariance kernel

$$m_n(x) = m(x) + k(x, \mathbf{X}_n)k(\mathbf{X}_n, \mathbf{X}_n)^{-1}(\mathbf{f}_n - m(\mathbf{X}_n))$$

$$k_n(x, y) = k(x, y) - k(x, \mathbf{X}_n)k(\mathbf{X}_n, \mathbf{X}_n)^{-1}k(\mathbf{X}_n, y)$$

 Γ^{\star} is a realization of $\Gamma = \{x \in D : Z_x \leq t\} = Z^{-1}((-\infty, t])$

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A prior on the space of functions

Assume: f realization of $(Z_x)_{x \in D}$, Gaussian Random Field (GRF)



Prior: $(Z_x)_{x \in D}$ with

- a.s. continuous paths;
- Matérn covariance kernel k ($\nu = 3/2$);
- constant mean function m.

Given n = 15 evaluations \mathbf{f}_n at \mathbf{X}_n

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Conclusio

Distribution of excursion sets

The posterior field induces a posterior distribution on excursion sets.



Excursion set realization

Note that

- Z continuous paths;
- $(-\infty, t]$ is a closed set.

Conservative estimates

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The set $\Gamma = \{x \in D : Z_x \leq t\}$ is a random closed set.

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How to summarize the distribution on sets?

Here we consider the computational challenges associated with

Estimates for Γ^* with

- **Expectations** of random closed sets¹, (*Vorob'ev expectation*).
- Conservative estimates, based on Vorob'ev quantiles.

Reduce the uncertainties on excursion set estimates.

Visualization of the excursion set with profile extrema functions.

1. for more definitions of expectation see Molchanov, I. (2005). Theory of Random Sets. Springer.

Conservative estimate

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Vorob'ev quantiles and Conservative estimates Computational issues GanMC method

SUR strategies for conservative estimates

Sequential strategies IRSN test case

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Vorob'ev quantiles

The function $p_n : x \in D \rightarrow p_n(x) = P_n(x \in \Gamma) \in [0, 1]$ is the **coverage** function of Γ , where $P_n(\cdot) = P(\cdot | Z_{\mathbf{X}_n} = \mathbf{f}_n)$.



In the Gaussian case

•
$$p_n(x) = \Phi\left(\frac{t-m_n(x)}{\sqrt{k_n(x,x)}}\right)$$

- creates a family of set estimates $Q_{\rho} = \{x \in D : p_n(x) \ge \rho\}$
- high ρ, then points in Q_ρ have high marginal probability.

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Vorob'ev quantiles

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In the Gaussian case

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- creates a family of set estimates $Q_{\rho} = \{x \in D : p_n(x) \ge \rho\}$
- high ρ, then points in Q_ρ have high marginal probability.
- Vorob'ev expectation: choose $Q_{\tilde{\rho}}$ such that $\mu(Q_{\tilde{\rho}}) = \mathbb{E}[\mu(\Gamma)]$. See Chevalier et al (2013).

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A conservative estimate of Γ^* is

$$\mathcal{C}_{\Gamma,n} = \mathcal{Q}_{
ho^*} ext{ where }
ho^* \in rgmax_{
ho\in[0,1]} \{\mu(\mathcal{Q}_{
ho}): \mathcal{P}_n(\mathcal{Q}_{
ho}\subset\Gamma)\geq lpha\}$$



- joint confidence statement on the set estimate;
- method introduced for Gauss Markov random fields, expensive to compute otherwise.
- computational bottleneck: estimation of P_n(Q_ρ ⊂ Γ).

Bolin, D. and Lindgren, F. (2015). *Excursion and contour uncertainty regions for latent Gaussian models.* JRSS: B, 77(1):85-106.

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The computation of conservative estimates

The family of sets Q_{ρ} is *nested*, therefore we can obtain $C_{\Gamma,n}$ with a **dichotomy on the level** ρ .

At each iteration of the dichotomy we need to compute

$$P_n(Q_\rho \subset \Gamma) = P_n(Q_\rho \subset \{Z_x \leq t\}) = P_n(Z_{e_1} \leq t, \ldots, Z_{e_k} \leq t),$$

where $E = \{e_1, \ldots, e_k\}$ is a the discretization of Q_{ρ} .

- randomized quasi Monte Carlo integration by Genz et al. : (Fast, reliable, dimension dependent, available only k < 1000)
- standard Monte Carlo.

(dimension independent, many samples for low variance)
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A quasi Monte Carlo algorithm for orthant probabilities

Candidate p = 0.95

$$P_n(Q_\rho \subset \{Z_x \le t\}) =$$

$$P_n(Z_{e_1} \le t, \dots, Z_{e_k} \le t) =$$

$$1 - P_n(\max_{x \in E} Z_x > t) = 1 - p$$

Main idea: $p = P_n(\max_E Z_x > t) = p_q + (1 - p_q)R_q$, where

 $\begin{array}{ll} p_q = P_n(\max_{E_q} Z_x > t), \qquad R_q = P_n(\max_{E \setminus E_q} Z_x > t \mid \max_{E_q} Z_x \leq t). \\ \text{Genz algorithm (QRSVN)} & \text{Monte Carlo methods} \end{array}$

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A quasi Monte Carlo algorithm for orthant probabilities



$$P_n(Q_\rho \subset \{Z_x \le t\}) =$$

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Main idea: $p = P_n(\max_E Z_x > t) = p_q + (1 - p_q)R_q$, where

| $p_q = P_n(\max_{E_q} Z_x > t),$ | $R_q = P_n(\max_{E \setminus E_q} Z_x > t \mid \max_{E_q} Z_x \leq t).$ | | |
|----------------------------------|---|--|--|
| Genz algorithm (QRSVN) | Monte Carlo methods More | | |
| $\widehat{p_q} = 0.47$ | $\widehat{R_q} = 0.42 \qquad \Rightarrow \widehat{p} = 0.69$ | | |

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Computation of the remainder

 $R_q = P_n(\max_{E \setminus E_q} Z_x > t \mid \max_{E_q} Z_x \leq t)$

Standard Monte Carlo:

- 1. draw realizations z_1^q, \ldots, z_s^q from $Z_{E_q} \mid \max_{E_q} Z_x \leq t$;
- 2. for each z_i^q , draw a realization from $Z_{E \setminus E_q} \mid Z_{E_q} = z_i^q$;
- 3. Estimate R_q with $R_q^{MC} = \frac{1}{s} \sum_{i=1}^{s} \mathbf{1}_{\max(Z_{E \setminus E_q}(\omega_i) | Z_{E_q} = z_i^q) > t}$

The cost of step 1 is higher than the cost of step 2.

At fixed computational budget we reduce the variance of R_q^{MC} exploiting this difference with **asymmetric nested Monte Carlo**.

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Computation of the remainder

At fixed computational budget we reduce the variance of R_q^{MC} drawing many realizations of $Z_{E \setminus E_q} \mid Z_{E_q} = z_i^q$ for each z_i .



Standard marginal/conditional scheme

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Computation of the remainder

At fixed computational budget we reduce the variance of R_q^{MC} drawing many realizations of $Z_{E \setminus E_q} \mid Z_{E_q} = z_i^q$ for each z_i .



Standard marginal/conditional scheme

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Computation of the remainder

At fixed computational budget we reduce the variance of R_q^{MC} drawing many realizations of $Z_{E \setminus E_q} \mid Z_{E_q} = z_i^q$ for each z_i .



Asymmetric sampling scheme

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Computation of the remainder: asymmetric nested MC

 $R_q = P_n(\max_{E \setminus E_q} Z_x > t \mid \max_{E_q} Z_x \le t)$

1. draw realizations z_1^q, \ldots, z_s^q from $Z_{E_q} \mid \max_{E_q} Z_x \leq t$;

2. for each z_i^q , draw $m^* > 1$ samples from $Z_{E \setminus E_q} \mid Z_{E_q} = z_i^q$;

3.
$$R_q^{\text{anMC}} = \frac{1}{s} \frac{1}{m^*} \sum_{i=1}^s \sum_{j=1}^{m^*} \mathbf{1}_{\max(Z_E \setminus E_q(\omega_{i,j}) | Z_{E_q} = z_i^q) > t}$$

 $\operatorname{var}(R_q^{\operatorname{anMC}})$ is optimally reduced if: $m^* = \sqrt{\frac{(\alpha+c)B}{\beta(A-B)}}$, where $A = \operatorname{var}(\mathbf{1}_{\max(Z_{E \setminus E_q} | Z_{E_q}) > t})$, $B = \mathbb{E}[\operatorname{var}(\mathbf{1}_{\max(Z_{E \setminus E_q} | Z_{E_q}) > t} | \max_{E_q} Z_x \leq t)]$ and α, β, c system dependent constants. More

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Comparison with standard Monte Carlo

Conservative estimate at 95%



Full discretization: grid 100×100

Dimension of candidate sets between 971 and 2370.

Time for equivalent estimates:

- Full MC: 1520 seconds;
- GMC: 200 seconds;
- GanMC: 136 seconds.

A., D. and Ginsbourger D. (2018). Estimating orthant probabilities of high dimensional Gaussian vectors with an application to set estimation. J. Comput. Graph. Statist., 27(2):255267. hal-01289126

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Sequential strategies for uncertainty reduction

Sequential design of experiments: sequentially evaluate f at points that minimize a specific acquisition function.

Stepwise uncertainty reduction strategies: find a sequence of evaluation points X_1, X_2, \ldots that optimally reduces the expected uncertainty on the future estimate, i.e. given an initial design X_n , select

$$X_{n+1} \in \arg\min_{x_{n+1} \in D} \mathbb{E}_n[H_{n+1} \mid X_{n+1} = x_{n+1}]$$

Issues:

- define appropriate uncertainty functions for set estimates;
- minimize the expected uncertainty.

Bect, J., Bachoc, F., and Ginsbourger, D. (2018+). A supermartingale approach to Gaussian process based sequential design of experiments. hal-01351088.

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Example



- Initial design, n = 10, maximin LHS
- constant mean function
- Matérn $\nu = 3/2$ covariance
- threshold t = 1
- Vorob'ev and conservative estimates.

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How to reduce the uncertainty on the estimate?

Uncertainty function(s): many possible definitions

$$\begin{split} & \mathcal{H}_n(\rho) = \mathbb{E}_n[\mu(\Gamma \Delta Q_{n,\rho})], \quad \Gamma \Delta Q_{n,\rho} = \Gamma \setminus Q_{n,\rho} \cup Q_{n,\rho} \setminus \Gamma, \\ & \mathcal{H}_n^{\text{T2}}(\rho_n^{\alpha}) = \mathbb{E}_n[\mu(\Gamma \setminus Q_{n,\rho_n^{\alpha}})], \end{split}$$

For each uncertainty function, we define the following SUR criteria

$$J_{n}(x) = \mathbb{E}_{n}[H_{n+1}(\rho) \mid X_{n+1} = x] = \mathbb{E}_{n}[\mu(\Gamma \Delta Q_{n+1,\rho}) \mid X_{n+1} = x]$$
$$J_{n}^{T2}(x) = \mathbb{E}_{n}[H_{n+1}^{T2}(\rho_{n}^{\alpha}) \mid X_{n+1} = x] = \mathbb{E}_{n}[\mu(\Gamma \setminus Q_{n+1,\rho_{n}^{\alpha}}) \mid X_{n+1} = x],$$

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Example: T2 criterion



More

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Example: T2 criterion



More

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Example: T2 criterion



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Example: T2 criterion



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Example: T2 criterion



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IRSN test case



Test case:

- k_{eff} function of PuO_2 density and H_2O thickness, $D = [0.2, 5.2] \times [0, 5]$;
- $k_{\rm eff}$ continuous, expensive to evaluate;
- *n* = 20 observations (black triangles);

Objective: estimate $\Gamma^* = \{x \in D : f(x) \le t\}$ and evaluate the uncertainty of the estimate.

GRF model: *m* constant, *k* Matérn $(\nu = 5/2)$, MLE for hyper-parameters.

Acknowledgements: Yann Richet, Institut de Radioprotection et de Sûreté Nucleaire.

Conservative estimate

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IRSN test case



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IRSN test case: type II uncertainty

Initial design, conservative Estimate



IRSN test case: type II uncertainty

Iteration 1, conservative Estimate



IRSN test case: type II uncertainty

Iteration 2, conservative Estimate



IRSN test case: type II uncertainty

Iteration 3, conservative Estimate



IRSN test case: type II uncertainty

Iteration 4, conservative Estimate



IRSN test case: type II uncertainty

Iteration 5, conservative Estimate



IRSN test case: type II uncertainty

Iteration 6, conservative Estimate



IRSN test case: type II uncertainty

Iteration 7, conservative Estimate



IRSN test case: type II uncertainty

Iteration 8, conservative Estimate



IRSN test case: type II uncertainty

Iteration 9, conservative Estimate



IRSN test case: type II uncertainty

Iteration 10, conservative Estimate



IRSN test case: type II uncertainty

Iteration 11, conservative Estimate


IRSN test case: type II uncertainty

Iteration 12, conservative Estimate



IRSN test case: type II uncertainty

Iteration 13, conservative Estimate



IRSN test case: type II uncertainty

Iteration 14, conservative Estimate



IRSN test case: type II uncertainty

Iteration 15, conservative Estimate



IRSN test case: type II uncertainty

Iteration 16, conservative Estimate



IRSN test case: type II uncertainty

Iteration 17, conservative Estimate



IRSN test case: type II uncertainty

Iteration 18, conservative Estimate



IRSN test case: type II uncertainty

Iteration 19, conservative Estimate



IRSN test case: type II uncertainty

Iteration 20, conservative Estimate



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IRSN test case: Type II uncertainty

Iteration 20, conservative Estimate



n = 60 new evaluations;

Next evaluation chosen in order to minimize criterion J_n^{T2} ;

Volume of updated CE: 21.30 (true excursion: 22.04, initial estimate: 18.10)

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Comparison with state-of-the-art

IRSN test case: *m* constant, *k* Matérn ($\nu = 5/2$).



A., D., Ginsbourger, D., Chevalier, C., Bect, J. and Richet, Y. (2017+). Adaptive design of experiments for conservative estimation of excursion sets. Under revision. hal-01379642.

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Sequential strategies IRSN test case

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Visualization techniques

Problem: how to visualize sets in dimensions higher than 3?

For high dimensional data

- dimensionality reduction methods (PCA, multidimensional scaling, ...)
- projection pursuit, Tours
- parallel coordinates
- pair plots

Those methods are well suited for sets of points, however we lose the concept of set and often the boundaries are deformed.

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Visualization of excursion sets

Focus on excursion sets of the form

$$\Gamma = \{x \in D : f(x) \ge t\}$$

where $D \subset \mathbb{R}^d$, with $d \geq 3$.

Coordinate profile extrema functions

Consider, for $i \in \{1, ..., d\}$, \mathbf{e}_i , the *i*-th canonical coordinate vector. The *i*-th coordinate profile extrema functions are

$$\begin{array}{ll} \mathcal{P}_{i}^{\sup}\gamma: \ \eta \in \mathcal{E}_{\mathbf{e}_{i}} \longrightarrow \ \mathcal{P}_{i}^{\sup}\gamma(\eta) := \sup_{x_{i}=\eta}\gamma(\mathbf{x}) \\ \mathcal{P}_{i}^{\inf}\gamma: \ \eta \in \mathcal{E}_{\mathbf{e}_{i}} \longrightarrow \ \mathcal{P}_{i}^{\inf}\gamma(\eta) := \inf_{x_{i}=\eta}\gamma(\mathbf{x}). \end{array}$$

where $E_{\mathbf{e}_i} = \{\eta \in \mathbb{R} : \mathbf{e}_i^T \mathbf{x} = \eta, \mathbf{x} \in D\}$ and $\mathbf{x} = (x_1, \dots, x_i, \dots, x_d)$.

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Analytical test case

$$\gamma(\mathbf{x}) = \sin\left(a\mathbf{v_1}^T\mathbf{x} + b\right) + \cos\left(c\mathbf{v_2}^T\mathbf{x} + d\right) \qquad \mathbf{x} \in [0, 1]^2, \ \mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^2$$

where $a, b, c, d \in \mathbb{R}$, $\mathbf{v_1} = [\cos(\theta), \sin(\theta)]^T$, $\mathbf{v_2} = [\cos(\theta + \pi/2), \sin(\theta + \pi/2)]^T$ and $\theta = \pi/6$. Threshold t = 0.

Test function and coordinate profile extrema

Coordinate X1





Coordinate X2



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Conclusion

A generalization

Profile extrema functions

Consider for a fixed matrix $\Psi \in \mathbb{R}^{d \times p}$ the functions

$$P_{\Psi}^{sup}f(\eta) = \sup_{x:\Psi^{T}x=\eta} f(x) \qquad \qquad P_{\Psi}^{inf}f(\eta) = \inf_{x:\Psi^{T}x=\eta} f(x),$$

- In the previous example, with Ψ = v₁ ∈ ℝ² then P^{sup}_Ψf(η) is the sup of f under the constraint v^Tx = η.
- If d > 2 we can consider *bivariate profile extrema* where $\Psi \in \mathbb{R}^{d \times 2}$.

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Oblique profile extrema



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Profile extrema functions on posterior mean

Consider the analytical test case above, assume that only n = 20evaluations are available.

Model: GP with prior constant mean, Matern covariance kernel with $\nu = 5/2$, n = 20 points. MLE for hyper-parameters.

Set of interest: $\Gamma = \{x \in D : m_n(x) \ge t\}$ with t = 0.



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Evaluate the uncertainty on profile extrema

• Approximated posterior realizations

$$\widetilde{Z}_x = a(x) + \mathbf{b}^T(x)Z_E \quad (x \in D), \quad (1)$$

where $E = \{e_1, \ldots, e_m\}$, $a : D \longrightarrow \mathbb{R}$ is a trend function and $\mathbf{b} : D \longrightarrow \mathbb{R}^m$ is a vector-valued function of deterministic weights. More ;

- Compute profile extrema for each realization;
- Point-wise confidence intervals (red).
- probabilistic bound gives conservative confidence intervals (light blue) that account for approximation in eq. 1. More;



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Boucholeurs test case



Numerical simulations validated on flooding caused by Xynthia storm (BRGM). More

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Boucholeurs test case

 $(x_i, y_i) \in D \times \mathbb{R}$, i = 1, ..., n with $y_i = f(x_i)$. n = 200, $D = [0, 1]^5$. $f : D \subset \mathbb{R}^5 \to \mathbb{R}$ expensive to evaluate (around 30 mins).



Inputs:

Tide (x_1) : high tide level;

Surge (x_2) : the storm surge magnitude peak;

Phi (x_3) : phase difference tide and surge;

tMinus (x_4) : time duration surge increase;

tPlus (x_5) : time duration surge decrease;

Response: Number of cells flooded (25m). Square-root transformed.

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GP model

Model: Gaussian process with

•
$$n = 200;$$

• prior mean

$$m(\mathbf{x}) = c_0 + c_1 x_1 + c_2 x_2 + c_3 x_3^2 + c_4 x_4 + c_5 x_5.$$

• Matérn (
$$\nu = 3/2$$
) covariance kernel;

- unknown homogeneous noise estimated from data;
- MLE for hyper-parameters and trend.

Set of interest:
$$\Gamma = \{x \in D : m_n(x) \ge t\}$$
 with $t = \sqrt{1.2 \times 10^6 \text{ m}^2}$ and $t = \sqrt{6.5 \times 10^6 \text{ m}^2}$, where $D \subset \mathbb{R}^5$ and m_n posterior mean.

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Profile extrema functions (5-d)



Profile extrema:

- posterior mean (black solid);
- point-wise confidence intervals (90%, red).
- conservative bound ($\alpha = 5\%$, blue)

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Bivariate profile extrema





A., D., Ginsbourger, D., Rohmer, J., and Idier, D. (2018+). *Profile extrema for visualizing and quantifying uncertainties on excursion regions. Application to coastal flooding.* Technometrics, under review. arXiv:1710.00688.

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- Conservative estimates:
 - Reduced the computing time for conservative estimates;
 - Methods implemented in R package anMC.
- Sequential strategies for conservative estimates:
 - Stepwise Uncertainty Reduction framework;
 - Comparison with state-of-the-art strategies.
- Visualization of excursion regions with profile extrema:
 - analysis tool providing lower dimensional subsets of excursion;
 - Implemented in R package profExtrema

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Appendix

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SUR strategies formulae

Criterion J_n

The criterion J_n can be expanded in closed-form as

$$J_{n}(\mathbf{x}^{(q)};\rho_{n}) = \mathbb{E}_{n+q} \left[\mu \left(\Gamma \Delta Q_{n+q,\rho_{n}} \right) \mid X_{n+1} = \mathbf{x}_{1}^{(q)}, \dots, X_{n+q} = \mathbf{x}_{q}^{(q)} \right]$$
$$= \int_{D} \left(2\Phi_{2} \left(\begin{pmatrix} a_{n+q}(u) \\ \Phi^{-1}(\rho_{n}) - a_{n+q}(u) \end{pmatrix}; \begin{pmatrix} 1+\gamma_{n+q}(u) & -\gamma_{n+q}(u) \\ -\gamma_{n+q}(u) & \gamma_{n+q}(u) \end{pmatrix} \right)$$
$$- p_{n}(u) + \Phi \left(\frac{a_{n+q}(u) - \Phi^{-1}(\rho_{n})}{\sqrt{\gamma_{n+q}(u)}} \right) \right) d\mu(u), \text{ where}$$

$$a_{n+q}(u) = \frac{m_n(u) - t}{s_{n+q}(u)}, \quad \mathbf{b}_{n+q}(u) = \frac{K_q^{-1}k_n^T(u, \mathbf{x}^{(\mathbf{q})})}{s_{n+q}(u)}, \ \gamma_{n+q}(u) = \mathbf{b}_{n+q}^T(u)K_q\mathbf{b}_{n+q}(u),$$

with $u \in D$, $k_n(u, \mathbf{x}^{(\mathbf{q})}) = (k_n(u, x_{n+1}), \dots, k_n(u, x_{n+q}))$, $K_q = [k_n(x_{n+i}, x_{n+j})]_{i,j=1,\dots,q}, \Phi_2(\cdot; \Sigma)$ bivariate centred Normal distribution with covariance matrix Σ and $\Phi^{-1}(u)$ quantile at level u of the standard Normal distribution.

SUR strategies formulae

Criterion J_n^{T2}

The criterion $J_n^{T2}(\cdot; \rho_n^{\alpha})$ can be expanded in closed-form as

$$\begin{aligned} J_n^{T2}(\mathbf{x}^{(\mathbf{q})};\rho_n^{\alpha}) &= \mathbb{E}_{n+q} \left[G_n^{(2)}(Q_{n+q,\rho_n^{\alpha}}) \mid X_{n+1} = \mathbf{x}_1^{(\mathbf{q})}, \dots, X_{n+q} = \mathbf{x}_q^{(\mathbf{q})} \right] \\ &= \int_D \Phi_2 \left(\begin{pmatrix} a_{n+q}(u) \\ \Phi^{-1}(\rho_n^{\alpha}) - a_{n+q}(u) \end{pmatrix}; \begin{pmatrix} 1+\gamma_{n+q}(u) & -\gamma_{n+q}(u) \\ -\gamma_{n+q}(u) & \gamma_{n+q}(u) \end{pmatrix} \right) d\mu(u) \end{aligned}$$

where

$$a_{n+q}(u) = \frac{m_n(u) - t}{s_{n+q}(u)}, \quad \mathbf{b}_{n+q}(u) = \frac{K_q^{-1}k_n^T(u, \mathbf{x}^{(\mathbf{q})})}{s_{n+q}(u)}, \ \gamma_{n+q}(u) = \mathbf{b}_{n+q}^T(u)K_q\mathbf{b}_{n+q}(u),$$

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with $u \in D$, $k_n(u, \mathbf{x}^{(\mathbf{q})}) = (k_n(u, x_{n+1}), \dots, k_n(u, x_{n+q}))$, $K_q = [k_n(x_{n+i}, x_{n+j})]_{i,j=1,\dots,q}, \Phi_2(\cdot; \Sigma)$ bivariate centred Normal distribution with covariance matrix Σ and $\Phi^{-1}(u)$ quantile at level u of the standard Normal distribution.

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