Sequential and batch-sequential Bayesian sampling strategies

for the identification of an excursion set

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supervised by David Ginsbourger (University of Bern) and
Yann Richet (IRSN)

Mascot-SAMO 2013, Ph.D. student day, Nice, July 1st 2013

Outline

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1. Motivations
2. SUR strategies for inversion, state of the art and contributions
3. SUR strategies for robust inversion

Problem description

Context

Let us consider an expensive-to-evaluate black box simulator f:

$$f : \mathbb{X} \subset \mathbb{R}^d \longmapsto \mathbb{R}$$

$$\boldsymbol{x} \longmapsto f(\boldsymbol{x})$$

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- Evaluating $f(\boldsymbol{x})$ at one point $\boldsymbol{x} \in \mathbb{X}$ takes a lot of time.
- Very small budget to evaluate f.

Motivations
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Identify the excursion set: $\Gamma^{\star}_{\text{inversion}} := \{\boldsymbol{x} \in \mathbb{X} : f(\boldsymbol{x}) \geq T\}$

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Among the d inputs, d_c are controlled and d_u are not. We want to identify the set:

$$\Gamma^\star_{\text{rob.inv}} := \{\boldsymbol{x}_c \in \mathbb{X}_c : \forall \boldsymbol{x}_u \in \mathbb{X}_u, f(\boldsymbol{x}_c, \boldsymbol{x}_u) \leq T\}$$

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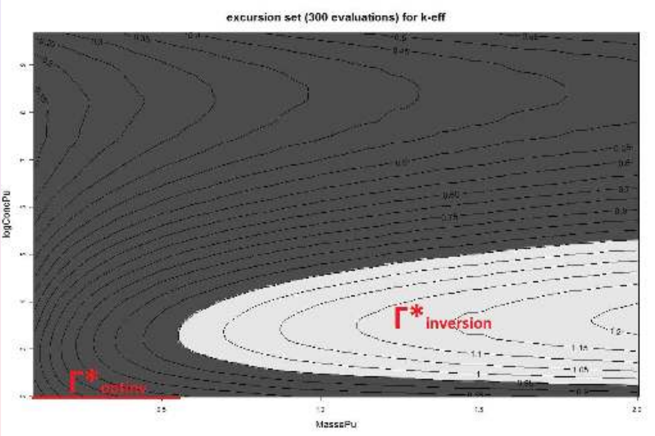
Our strategy will be based on a **Kriging** metamodel.

Motivations
Context



Kriging
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- Kriging mean: $m_n(\boldsymbol{x})$
- Kriging variance: $s_n^2(\boldsymbol{x})$
- $\mathcal{L}(\xi(\boldsymbol{x})|\mathcal{A}_n) = \mathcal{N}(m_n(\boldsymbol{x}), s_n^2(\boldsymbol{x}))$

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SUR strategies for inversion

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SUR strategies for inversion

Short description of a SUR strategy:

- Defining a measure of uncertainty for the problem at hand
- Optimal 1-step lookahead criterion: Expectation of the future uncertainty if an observation $\boldsymbol{x}_{n+1}$ is added.
- SUR strategy: sampling sequentially at the location where the criterion is minimized.

SUR strategies for inversion

Starting point:

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

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Set of interest:

$$\Gamma := \{\boldsymbol{x} \in \mathbb{X} : \xi(\boldsymbol{x}) \geq T\}$$

Uncertainty:

$$H_n := Var_n(\mathbb{P}_{\mathbb{X}}(\Gamma))$$

SUR strategies for inversion

In Bect et. al., the uncertainty H_n is judged intractable so that a different definition of the uncertainty is used:

$$H_n \leq \widetilde{H}_n := \int_{\mathbb{X}} p_n(1 - p_n) \mathrm{d}\mathbb{P}_{\mathbb{X}}$$

where

$$\begin{aligned} p_n(\boldsymbol{x}) :=& P(\boldsymbol{x} \in \Gamma | \mathcal{A}_n) \\ =& P(\xi(\boldsymbol{x}) \geq T | \mathcal{A}_n) \end{aligned}$$

The function $p_n(\cdot)$ is called excursion (or coverage) probability function

SUR strategies for inversion

The optimal one-step lookahead SUR criteria that need to be minimized to find the next evaluation location are:

$$J_n(\mathbf{x}) := \mathbb{E}_n(H_{n+1} | X_{n+1} = \mathbf{x})$$
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Main issue with SUR strategies:

- Computer intensive
- Designed to sample one point at a time, whereas we often have $r > 1$ CPUs to evaluate f in parallel.
- **A first contribution:** definition of a **multi-points** generalization of the SUR criteria and "fast" formulas to compute both the one-point and multi-points version of J_n and $\widetilde{J}_n$.

SUR strategies for inversion

Proposition (1)

$$\widetilde{J}_n(\boldsymbol{x}^{(r)}) = \int_{\mathbb{X}} \Phi_2\left(\begin{pmatrix} a(\boldsymbol{x}) \\ -a(\boldsymbol{x}) \end{pmatrix}, \begin{pmatrix} c(\boldsymbol{x}) & 1-c(\boldsymbol{x}) \\ 1-c(\boldsymbol{x}) & c(\boldsymbol{x}) \end{pmatrix} \right) \mathrm{d}\mathbb{P}_{\mathbb{X}}(\boldsymbol{x}),$$

$$J_n(\boldsymbol{x}^{(r)}) = \gamma_n - \int_{\mathbb{X}\times\mathbb{X}} \Phi_2\left(\begin{pmatrix} a(z_1) \\ -a(z_2) \end{pmatrix}, \begin{pmatrix} c(z_1) & d(z_1,z_2) \\ d(z_1,z_2) & c(z_2) \end{pmatrix} \right) \mathbb{P}_{\mathbb{X}}(\mathrm{d}z_1)\mathbb{P}_{\mathbb{X}}(\mathrm{d}z_2)$$

- $\Phi_2(\cdot, M)$ *is the c.d.f. of the centered bivariate Gaussian with covariance matrix* M
- $a(\boldsymbol{x}) := (m_n(\boldsymbol{x}) - T)/s_{n+r}(\boldsymbol{x}),$
- $\mathbf{b}(\boldsymbol{x}) := \frac{1}{s_{n+r}(\boldsymbol{x})}\Sigma^{-1}(k_n(\boldsymbol{x},\boldsymbol{x}_{n+1}),\ldots,k_n(\boldsymbol{x},\boldsymbol{x}_{n+r}))^\top$
- $c(\boldsymbol{x}) := s_n^2(\boldsymbol{x})/s_{n+r}^2(\boldsymbol{x})$
- $d(z_1,z_2) := \mathbf{b}(z_1)^\top \Sigma\, \mathbf{b}(z_2)$
- Σ *is conditional covariance matrix of* $(\xi(\boldsymbol{x}_{n+1}),\ldots,\xi(\boldsymbol{x}_{n+r}))^\top$.
- γ_n *does not depend on* $(\boldsymbol{x}_{n+1},\ldots,\boldsymbol{x}_{n+r})$.

SUR strategies for inversion

Details and proofs can be found in:

C. C, J. Bect, D. Ginsbourger, E. Vazquez, V. Picheny and Y. Richet.
Fast parallel kriging-based stepwise uncertainty reduction with application to the identification of an excursion set.
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The proof widely rely on the “kriging update” formulas:

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A key step in the proof is to write the updated kriging mean function, $m_{n+r}(\cdot)$, as a function of the unknown response $\xi(\boldsymbol{x}^{(r)})$.

Applications
Nuclear Safety

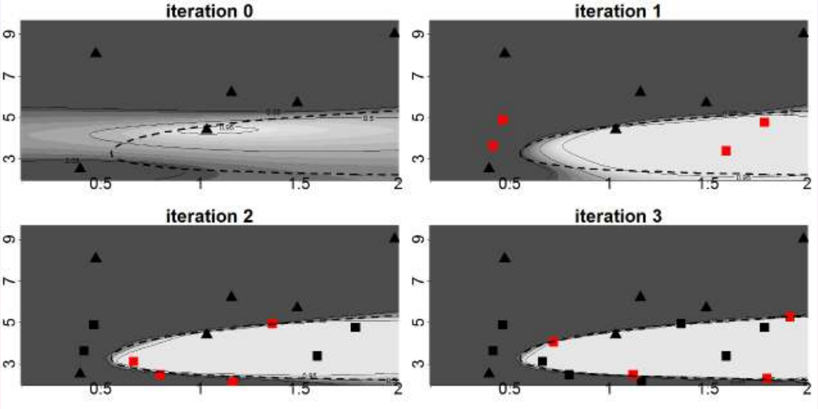

Figure: 3 iterations of a parallel SUR algorithm (criterion $\widetilde{J}_n$ with $r = 4$)

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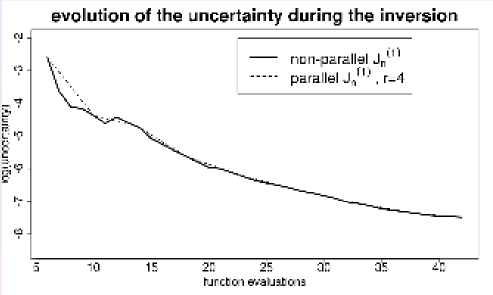

Figure: Evolution of $\int_{\mathbb{X}} p_n(1 - p_n)\mathrm{d}\mathbb{P}_{\mathbb{X}}$ during the inversion.

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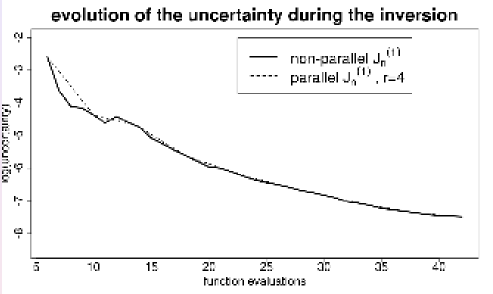

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The KrigInv package: An efficient and user-friendly R implementation of Kriging-based inversion algorithms.
Computational Statistics & Data Analysis, 2013

SUR strategies for inversion

Random sets

Motivation: the presented SUR strategies are meant to reduce the variance of the excursion's volume (or a bound of this volume).

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If we are interested in:

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we would like to define a "variance" for the random excursion set:

$$\Gamma := \{\boldsymbol{x} \in \mathbb{X} : \xi(\boldsymbol{x}) \geq T\}$$

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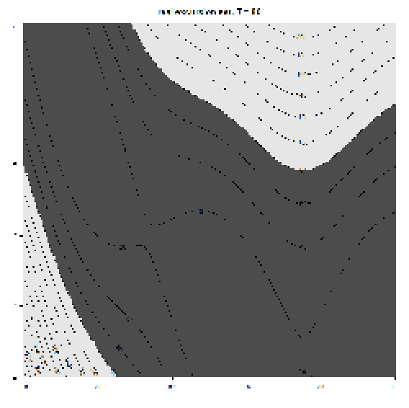

Figure: Real (unknown) excursion set of a two dimensional function, with a threshold $T = 80$.

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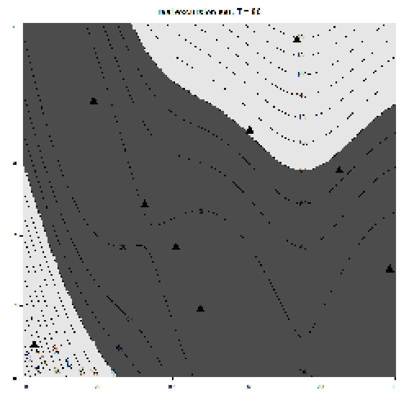

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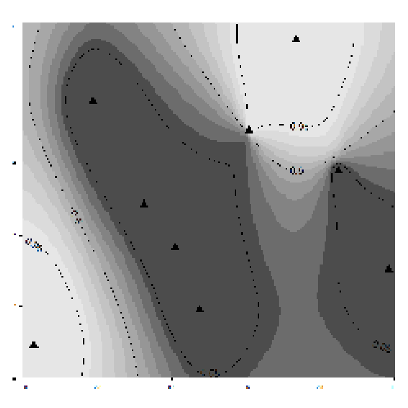

Figure: Coverage probability calculated using Kriging, on a two dimensional function, with a threshold $T = 80$.

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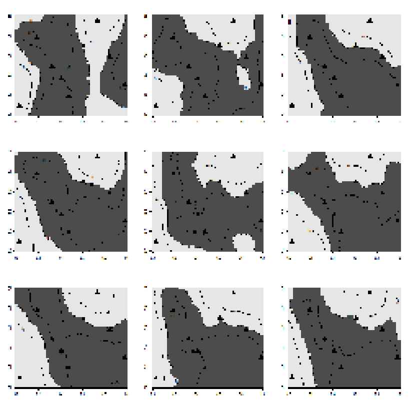

Figure: Random set realizations, obtained with GP conditional simulations.

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There exist different approaches to define the expectation and the variance of a random set.

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SUR strategies for inversion

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One of them is the Vorob'ev approach.

SUR strategies for inversion

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Vorob'ev expectation:

$$Q_{n,\alpha_n} := \{\boldsymbol{x} \in D : p_n(\boldsymbol{x}) \geq \alpha_n\},$$

SUR strategies for inversion

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Vorob'ev deviation, our "variance"

It is proven that, $\forall$ closed set S with $\mathbb{P}_{\mathbb{X}}(S) = \nu_n$,

$$\mathbb{E}_n(\mathbb{P}_{\mathbb{X}}(Q_{n,\alpha_n} \triangle \Gamma)) \leq \mathbb{E}_n(\mathbb{P}_{\mathbb{X}}(S \triangle \Gamma)).$$

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We can thus define our **variance of a random set**:

$$Var_n(\Gamma) := \mathbb{E}_n(\mathbb{P}_{\mathbb{X}}(Q_{n,\alpha_n} \triangle \Gamma))$$

SUR strategies for inversion

Random sets

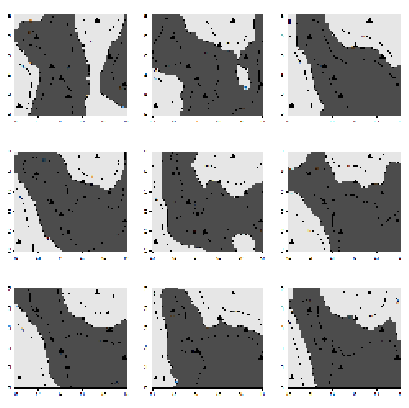
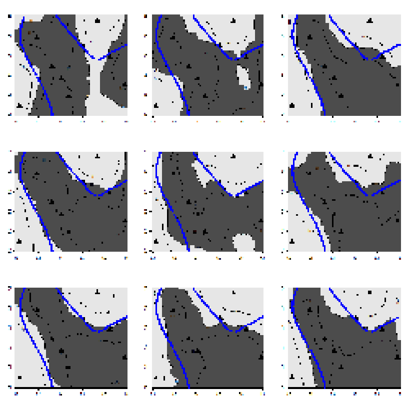


Figure: Random set realizations, obtained with GP conditional simulations.

SUR strategies for inversion
Random sets



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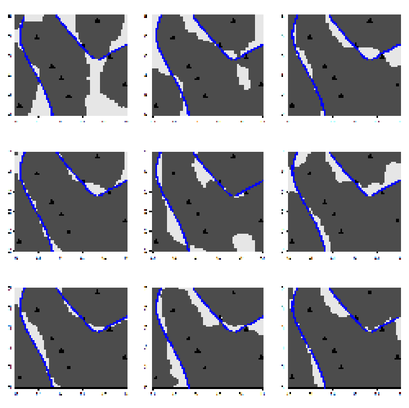

Figure: Symmetrical differences between the realizations and the Vorob'ev Expectation

SUR strategies for inversion

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Construction of a SUR strategy based on the uncertainty:

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SUR strategies for inversion
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Construction of a SUR strategy based on the uncertainty:

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- H_n can be computed quite easily.
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C. C, D. Ginsbourger, J. Bect and I. Molchanov
Estimating and quantifying uncertainties on level sets using the Vorob'ev expectation and deviance with Gaussian process models.
mODa 10, Advances in Model-Oriented Design and Analysis, Physica-Verlag HD, 2013.

Sequential sampling strategy

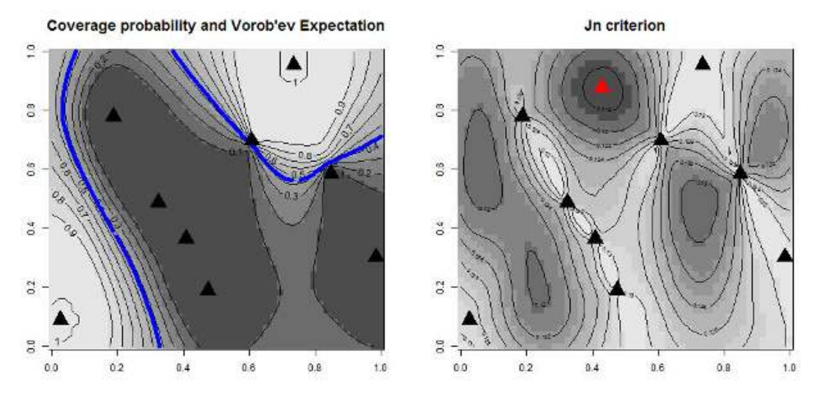

Figure: SUR sampling strategy reducing $Var_n(\Gamma)$. Iteration 0.

Sequential sampling strategy

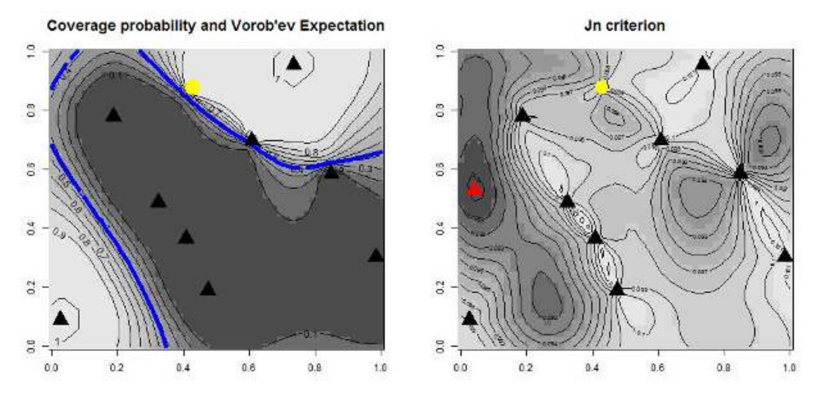

Figure: SUR sampling strategy reducing $Var_n(\Gamma)$. Iteration 1.

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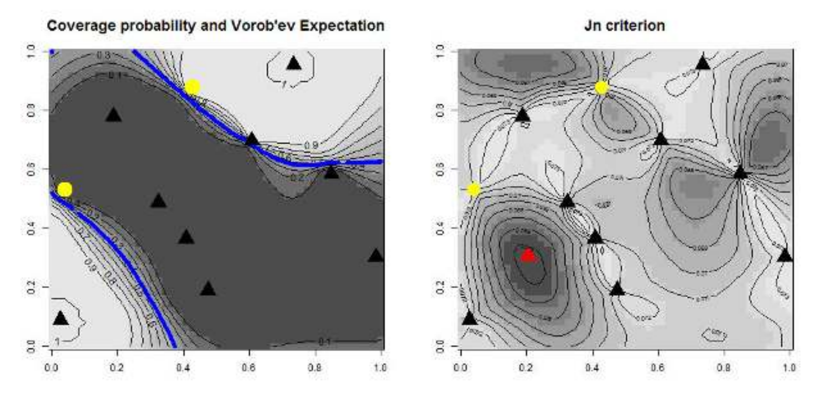

Figure: SUR sampling strategy reducing $Var_n(\Gamma)$. Iteration 2.

Sequential sampling strategy

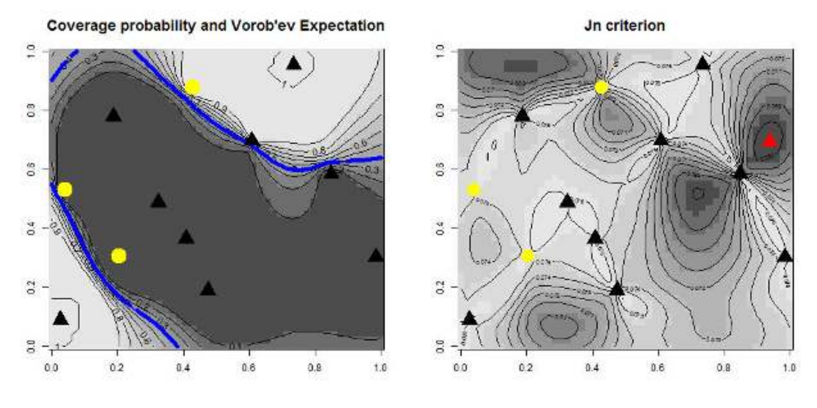

Figure: SUR sampling strategy reducing $Var_n(\Gamma)$. Iteration 3.

Sequential sampling strategy

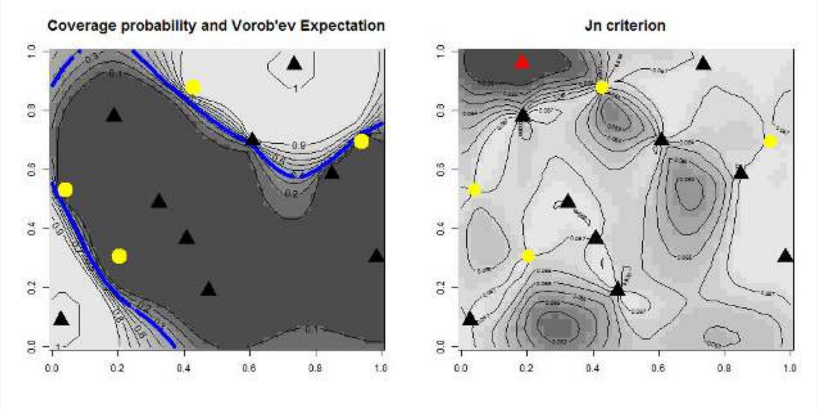

Figure: SUR sampling strategy reducing $Var_n(\Gamma)$. Iteration 4.

Sequential sampling strategy

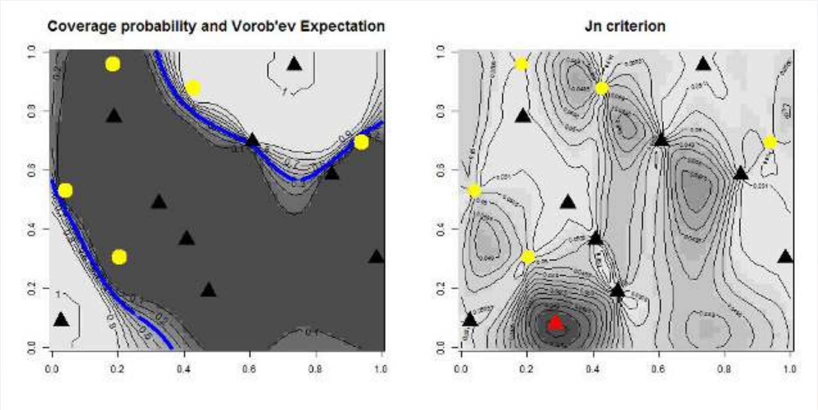

Figure: SUR sampling strategy reducing $Var_n(\Gamma)$. Iteration 5.

Sequential sampling strategy

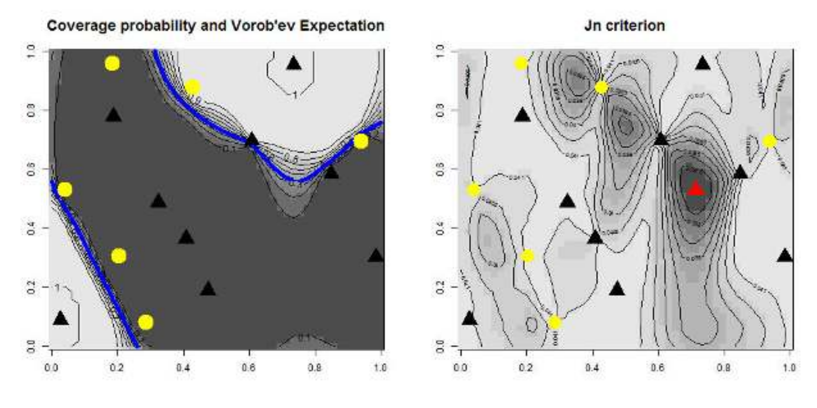

Figure: SUR sampling strategy reducing $Var_n(\Gamma)$. Iteration 6.

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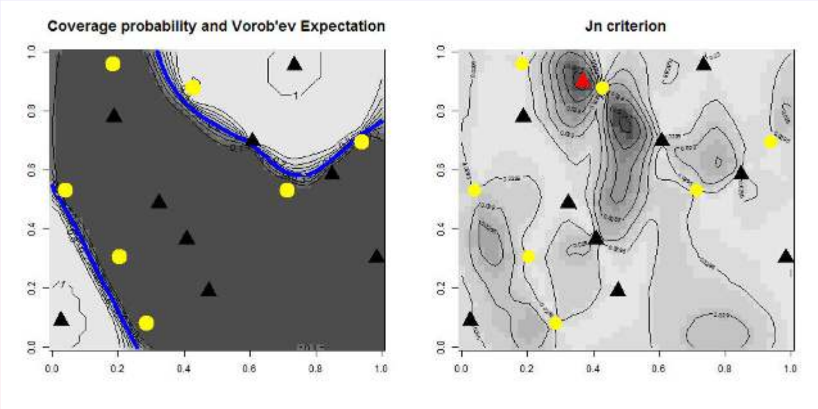

Figure: SUR sampling strategy reducing $Var_n(\Gamma)$. Iteration 7.

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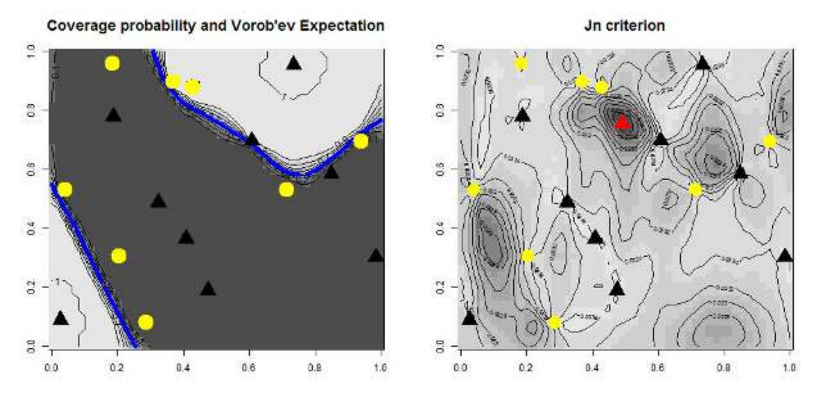


Figure: SUR sampling strategy reducing $Var_n(\Gamma)$. Iteration 8.

Sequential sampling strategy

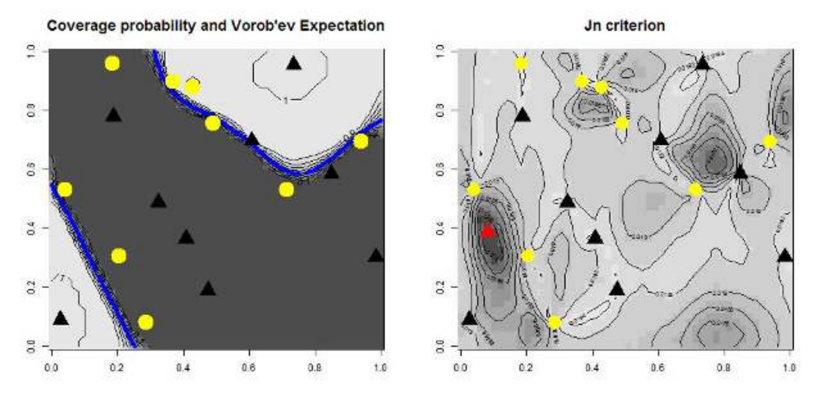
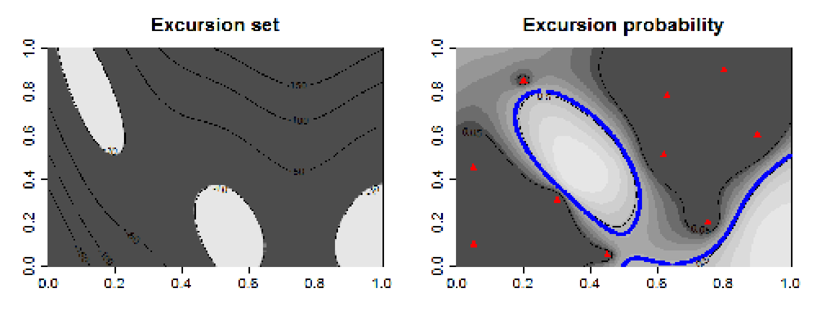
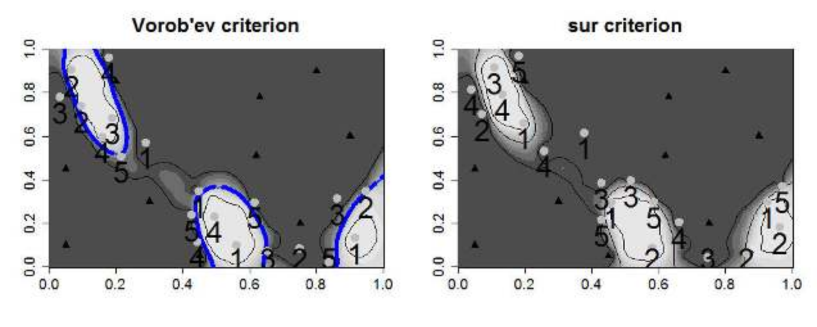


Figure: SUR sampling strategy reducing $Var_n(\Gamma)$. Iteration 9.

Sequential sampling strategy



Sequential sampling strategy



Outline

SUR strategies for robust inversion

In robust inversion, we aim at identifying the set:

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This set is a subset of $\mathbb{X}_c$.

SUR strategies for robust inversion

In robust inversion, we aim at identifying the set:

$$\Gamma^{\star}_{\text{optinv}} := \{\boldsymbol{x}_c \in \mathbb{X}_c : \forall \boldsymbol{x}_u \in \mathbb{X}_u, f(\boldsymbol{x}_c, \boldsymbol{x}_u) \leq T\}$$

This set is a subset of $\mathbb{X}_c$.

An uncertainty measure can be defined in the same spirit than in inversion.

SUR strategies for robust inversion

Excursion probability:

$$\widetilde{p_n}(\boldsymbol{x}_c) := P\left(\max_{\boldsymbol{x}_u \in \mathbb{X}_u} \xi(\boldsymbol{x}_c, \boldsymbol{x}_u) \leq T | \mathcal{A}_n\right)$$

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$$H_n := \int_{\mathbb{X}_c} \widetilde{p_n}(\boldsymbol{x}_c)(1 - \widetilde{p_n}(\boldsymbol{x}_c)) \mathrm{d}\mathbb{P}_{\mathbb{X}_c}(\boldsymbol{x}_c)$$

is a possible measure to quantify uncertainties on $\Gamma^{\star}_{\text{optinv}}$.

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is a possible measure to quantify uncertainties on $\Gamma^{\star}_{\text{optinv}}$.

Main issue

The associated SUR criterion is too expensive to compute !

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Goal: Find a “fast” approximation of $\widetilde{p_n}(\boldsymbol{x}_c)$.

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First idea

$$\widehat{p_n}(\boldsymbol{x}_c) := P\left(\max_{\boldsymbol{x}_u \in \{\boldsymbol{x}_u^{(1)},\ldots,\boldsymbol{x}_u^{(q)}\}} \xi(\boldsymbol{x}_c, \boldsymbol{x}_u) \leq T | \mathcal{A}_n\right)$$

where $\boldsymbol{x}_u^{(1)}, \ldots, \boldsymbol{x}_u^{(q)}$ are chosen so that $\widehat{p_n}(\boldsymbol{x}_c)$ is as close as possible to $\widetilde{p_n}(\boldsymbol{x}_c)$.

SUR strategies for robust inversion

The SUR criteria can be efficiently computed using a generalization of the results obtained in inversion:

$$J_n(\boldsymbol{x}^{(r)}) := \mathbb{E}_n\left(\int_{\mathbb{X}_c} \widehat{p_{n+r}}(\boldsymbol{x}_c)(1-\widehat{p_{n+r}}(\boldsymbol{x}_c))\mathrm{d}\mathbb{P}_{\mathbb{X}_c}(\boldsymbol{x}_c)\right)$$

$$= \int_{\mathbb{X}_c}\left(\widehat{p_n}(\boldsymbol{x}_c) - \Phi_{2q}\left(\begin{pmatrix}\mathbf{T}-\mathbf{m}_n^{(q)}\\ \mathbf{T}-\mathbf{m}_n^{(q)}\end{pmatrix}, \begin{pmatrix}\Sigma_n^{(q)} & B^\top\Sigma_n^{(r)}B\\ B^\top\Sigma_n^{(r)}B & \Sigma_n^{(q)}\end{pmatrix}\right)\right)\mathrm{d}\mathbb{P}_{\mathbb{X}_c}(\boldsymbol{x}_c)$$

SUR strategies for robust inversion

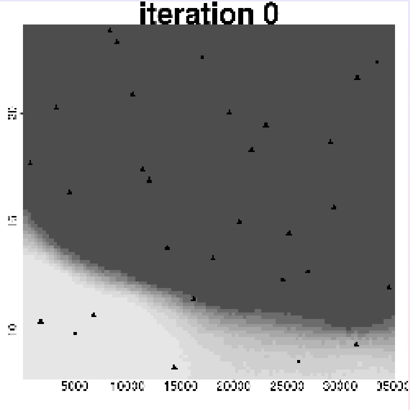
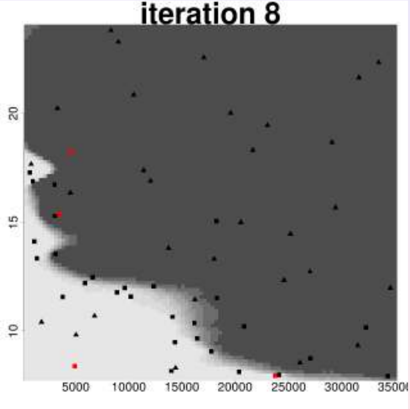


Figure: $\widehat{p}_n(\boldsymbol{x}_c)$ function at at current iteration.

SUR strategies for robust inversion



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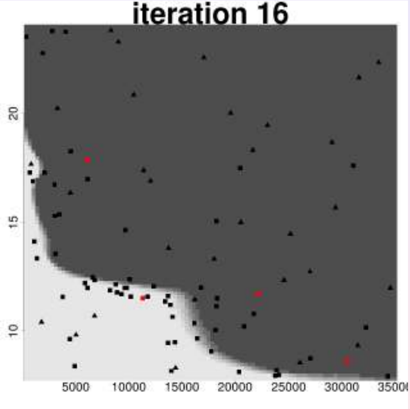

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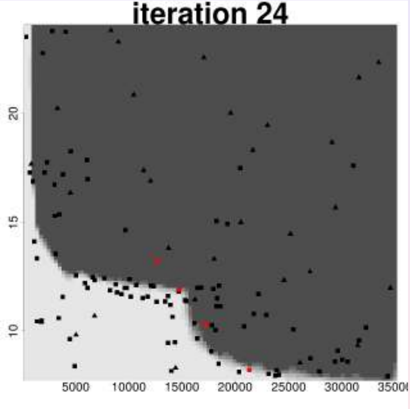

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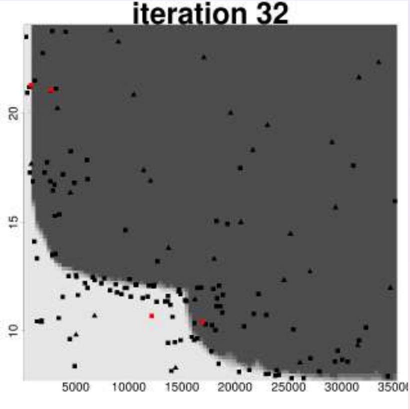

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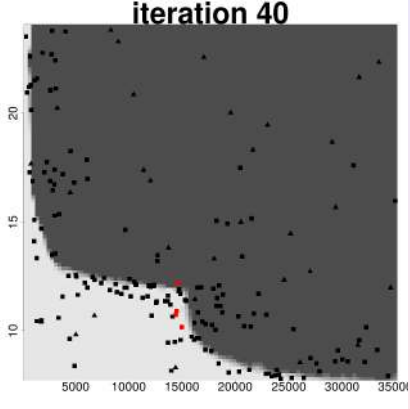

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Second idea: GP realization updates

$$\widehat{p_n}(\boldsymbol{x}_c) := \frac{1}{M} \# \{ i : \max_{1 \leq j \leq q} z^j_{i,n} \leq T \}$$

where $z^1_{i,n}, \ldots, z^q_{i,n}$ is a realization (conditioned on n obs.) of $\xi(\boldsymbol{x}_c, \cdot)$ in q locations.

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Idea: from the kriging update formulas, it is possible to calculate how a GP realization is modified by new observations.

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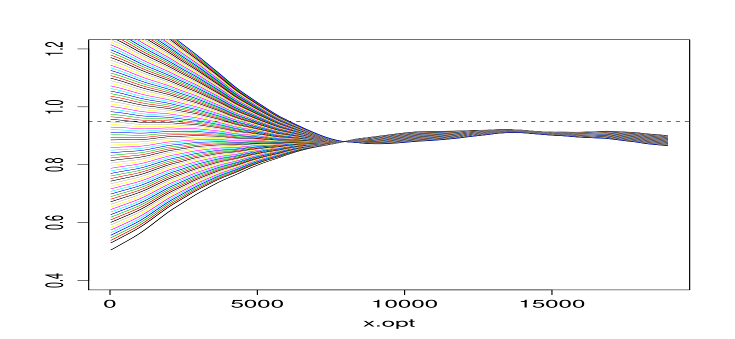

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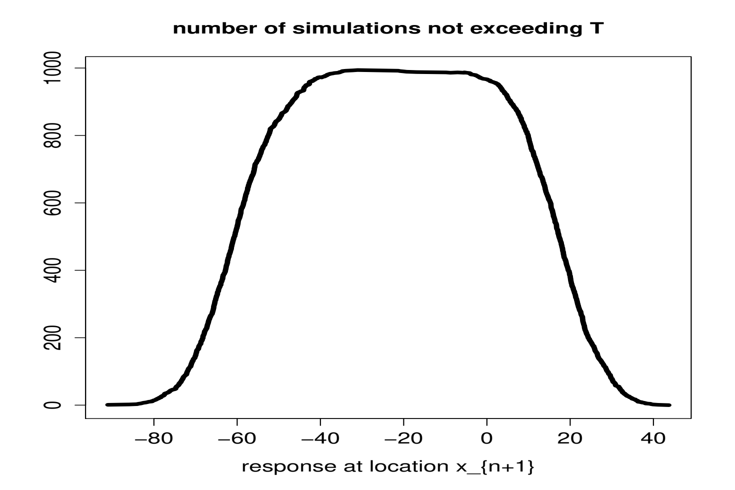

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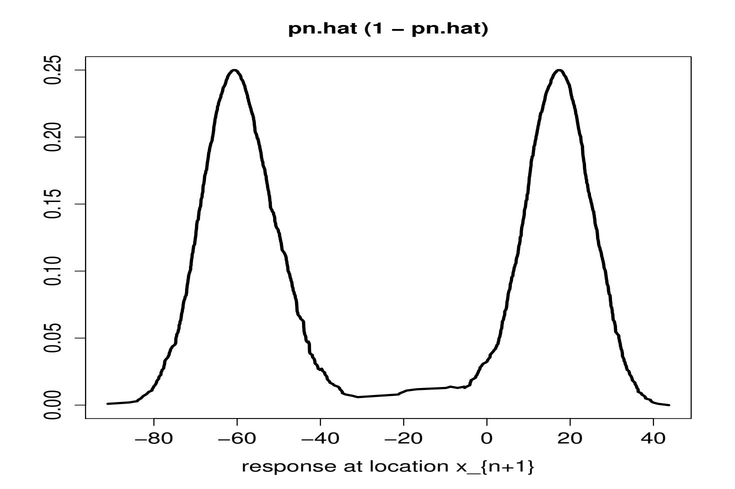

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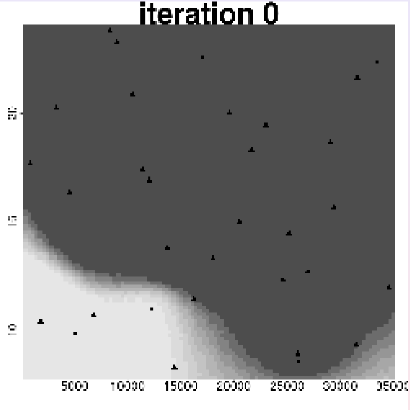

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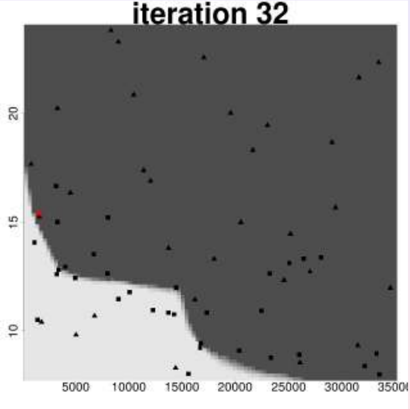

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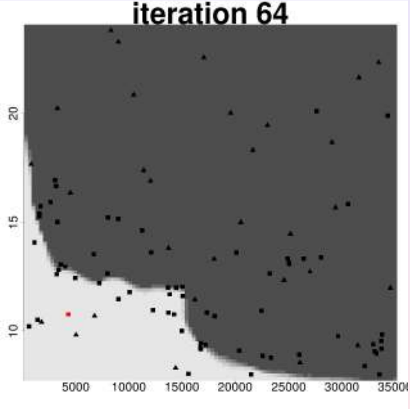

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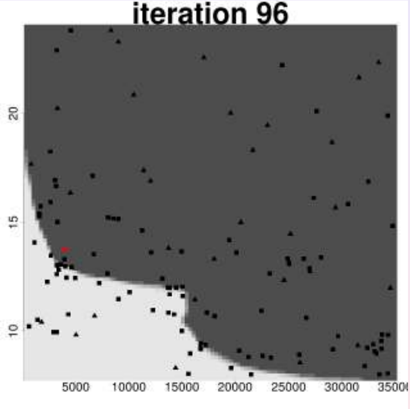

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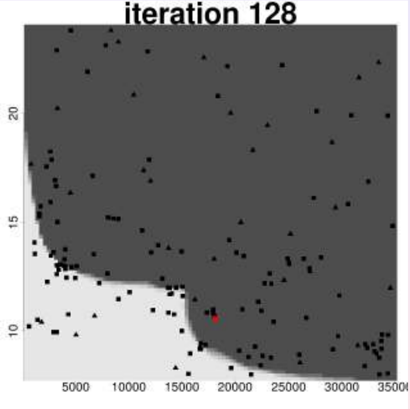

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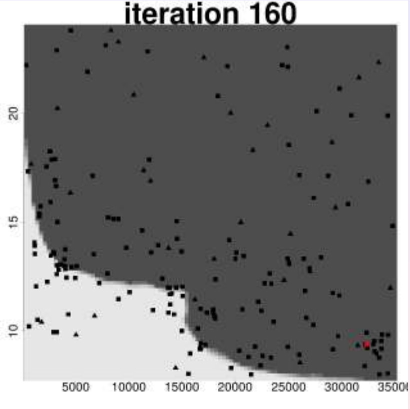

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Future work:

- Other approximations of the exceedance probability relying on e.g. the work of Adler and Taylor.

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- Other approximations of the exceedance probability relying on e.g. the work of Adler and Taylor.
- Convergence results.
- Choice of the integration points to compute the integrals: Sequential Monte-Carlo methods.

Future work

Thank you for your attention !

Future work

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any questions ?

Acknowledgement: Clément Chevalier acknowledges support from the IRSN and the ReDICE consortium.