A SUR adaptation of the Bichon criterion for inversion

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Introduction: Inversion framework

Excursion set to estimate

$$\Gamma^\star := \left\{\mathbf{x} \in \mathbb{X},\ g(\mathbf{x}) \leq T\right\} \tag{1}$$

with

- $\mathbb{X} \subset \mathbb{R}^d$ design space (compact)
- g "black-box" function (e.g. calculation run)
- T fixed threshold

Essential criterion to $\Gamma^\star$ estimation

- Limit the number of g's expensive simulations

Target application

- Floating wind turbine calibration
  - Estimation of fitting parameters to limit the error on site measurement (accelerations)

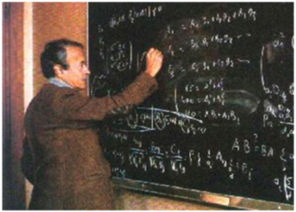
Introduction: Surrogate models and GP Regression

Surrogate models

- Approximation of the original model (simulator)
- Fast to evaluate
- Defined from a limited number of (expensive) simulations

Gaussian Process Regression (GPR)

- Hypothesis: g is a realization of a gaussian process (GP)
- Advantage: prediction error estimate



Professor Georges Matheron.

Sequential construction of a Design of Experiments (DoE) by GPR

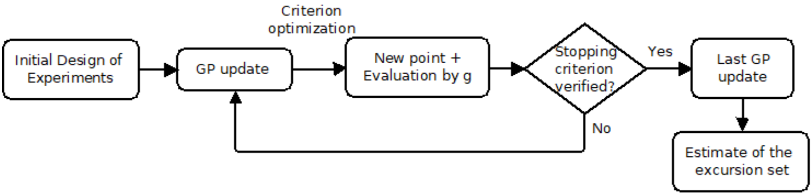


Figure 1: Functional diagram of the DoE sequential construction, by GPR.

Criterion choice

- Overall knowledge criteria (mse, IMSE, MMSE)
- Goal oriented criteria (*Picheny* [2010])
  - for optimization (EI, PI, ...)
  - for inversion (U, tmse, Bichon (EFF), Ranjan, SUR Vorob'ev , ...)

Introduction: Motivations of the work

Motivations

- SUR strategies show better performances than direct strategies (*Bect* [2012])
- SUR Vorob'ev may not be robust for disconnected excursion sets (see our numerical tests below)
- SUR Vorob'ev criterion requires approximations (see Appendix)
- Bichon criterion shows better performances than the Ranjan one (*Bect* [2012])

Goal

- Propose a SUR Bichon strategy:
  - more robust and easier to implement than SUR Vorob'ev one
  - with better performances than direct strategies

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Bichon criterion

Definition (*Bichon* [2008])

Reminder: Excursion set to estimate

$$\Gamma^\star := \left\{ \mathbf{x} \in \mathbb{X},\ g(\mathbf{x}) \leq T \right\} \tag{2}$$

with $\mathbb{X} \subset \mathbb{R}^d$ design space, g "black-box" function and T threshold

Notations

- $(\Omega, \mathscr{F}, \mathbb{P})$ a probability space
- $\xi(\mathbf{x})_{\mathbf{x}\in\mathbb{X}} \sim \mathrm{GP}(m, k)$: surrogate model
- $\mathscr{X}_n := (\mathbf{x}^{(1)}, ..., \mathbf{x}^{(n)})$: sequential DoE, $g(\mathscr{X}_n) := \left(g\left(\mathbf{x}^{(1)}\right), ..., g\left(\mathbf{x}^{(n)}\right)\right)$
- $\mathscr{E}_n := \left\{\xi(\mathscr{X}_n) = g(\mathscr{X}_n)\right\}$: event given by evaluations
- $m_n(\mathbf{x}) := \mathbb{E}\left[\xi(\mathbf{x}) \middle| \mathscr{E}_n\right]$
- $k_n(\mathbf{x}, \mathbf{x}') := \mathrm{Cov}\left[\xi(\mathbf{x}), \xi(\mathbf{x}') \middle| \mathscr{E}_n\right]$ and $\sigma_n(\mathbf{x}) := \sqrt{k_n(\mathbf{x}, \mathbf{x})}$

Bichon criterion

- Goal oriented criterion (adapted to inversion)

Enrichment of the DoE

$$\mathbf{x}^{(n+1)} := \underset{\mathbf{x}\in\mathbb{X}}{\operatorname{argmax}}\, \mathrm{EFF}(\mathbf{x}) \quad \text{with} \quad \mathrm{EFF}(\mathbf{x}) := \mathbb{E}\Big[\big(\varepsilon(\mathbf{x}) - |T - \xi(\mathbf{x})|\big)^+ \,\big|\, \mathscr{E}_n\Big] \quad (3)$$

with $\varepsilon(\mathbf{x}) := \kappa\sigma_n(\mathbf{x})$ and $\kappa > 0$

Feasibility Function

$$\begin{aligned} \mathrm{FF}(\mathbf{x}) &:= \big(\varepsilon(\mathbf{x}) - |T - \xi(\mathbf{x})|\big)^+ \\ &= \begin{cases} \varepsilon(\mathbf{x}) - |T - \xi(\mathbf{x})| & \text{if } \xi(\mathbf{x}) \in \big[T - \varepsilon(\mathbf{x}), T + \varepsilon(\mathbf{x})\big] \\ 0 & \text{otherwise} \end{cases} \end{aligned} \quad (4)$$

Interpretation

Interpretation of Feasibility Function

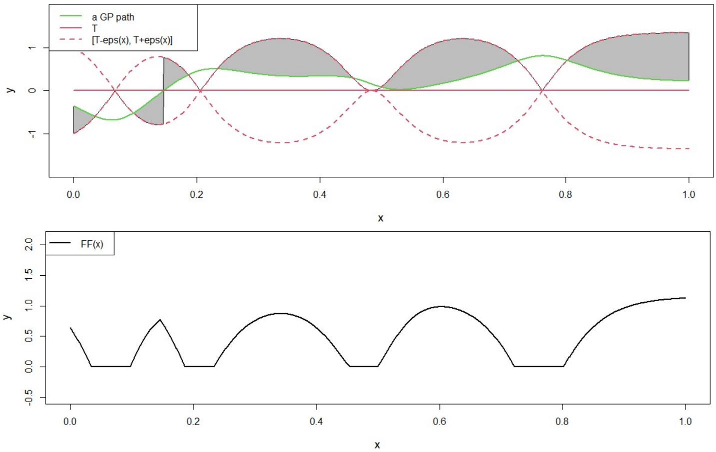

Figure 2: Representation of Feasibility Function for an example of a GP path.

SUR Strategies (Bect [2012])

Idea

- An adaptive strategy class
- Anticipate the impact of adding the next evaluation

SUR formulation

$$\mathbf{x}^{(n+1)} \in \arg\min_{\mathbf{x}\in\mathbb{X}} \mathscr{J}_n(\mathbf{x}) \quad \text{and} \quad \mathscr{J}_n(\mathbf{x}) := \mathbb{E}\left[\mathscr{H}_{n+1}(\mathbf{x})\right] \tag{5}$$

with

- $\mathscr{H}_{n+1}(\mathbf{x})$ a real random variable measurable with respect to $\xi(\mathbf{x})|\,\mathscr{E}_n$
- $\mathbf{x}^{(n+1)}$ new point to be added to the sequential DoE

Notation

- $\mathscr{H}_n$ uncertainty measure associated to $\mathscr{H}_{n+1}(\mathbf{x})$ with respect to $\mathscr{E}_n$ only

Example (*Chevalier* [2013])

- SUR Vorob'ev criterion:

$$\mathscr{H}_n^V := \mathbb{E}\left[\mathbb{P}_{\mathbb{X}}(\Gamma \Delta Q_{n,\alpha_n^\star}) \,\middle|\, \mathscr{E}_n\right] \tag{6}$$

  with
  - $\mathbb{P}_{\mathbb{X}}$ finite measure on $\mathbb{X}$
  - $\Gamma := \{\mathbf{x} \in \mathbb{X},\, \xi(\mathbf{x}) \leq T\}$
  - $Q_{n,\alpha_n^\star}$ Vorob'ev expectation (Appendix)
  - Δ symetric difference for random sets

Benefits of SUR strategies

- Better performances than direct strategies (*Bect* [2012])

Major problem of SUR strategies

- Explain the $\mathbf{x}$ dependence in the definition of $\mathscr{J}_n$ (equation (5))
  - Quadrature methods
  - Simplifying assumptions

SUR Bichon criterion

Definition and simplified formulation

Idea

- Propose a SUR version of the Bichon criterion
- Uncertainty measure: integral of the Bichon criterion on the design space

Definition

$$\mathscr{H}_n^{\mathrm{B}} := \int_{\mathbb{X}} \mathbb{E}\left[\left(\kappa\sigma_n(\mathbf{z}) - |T - \xi(\mathbf{z})|\right)^+ \,\middle|\, \mathscr{E}_n\right] \mathrm{d}\mathbb{P}_{\mathbb{X}}(\mathbf{z}) \left(= \int_{\mathbb{X}} \mathrm{EFF}(\mathbf{z})\, \mathrm{d}\mathbb{P}_{\mathbb{X}}(\mathbf{z})\right) \quad (7)$$

$$\mathscr{H}_{n+1}^{\mathrm{B}}(\mathbf{x}) := \int_{\mathbb{X}} \mathbb{E}\left[\left(\kappa\sigma_{n+1}(\mathbf{z}) - |T - \xi(\mathbf{z})|\right)^+ \,\middle|\, \xi(\mathbf{x}),\, \mathscr{E}_n\right] \mathrm{d}\mathbb{P}_{\mathbb{X}}(\mathbf{z}) \quad (8)$$

$$\mathscr{J}_n^{\mathrm{B}}(\mathbf{x}) := \mathbb{E}\left[\mathscr{H}_{n+1}^{\mathrm{B}}(\mathbf{x})\right] \quad (9)$$

with σ_{n+1} prediction standard deviation with the addition of $\mathbf{x}$ to the DoE (independent of the evaluation)

Simplified formulation

$$\mathscr{J}_n^{\mathrm{B}}(\mathbf{x}) = \int_{\mathbb{X}} \mathrm{EFF}_{\mathbf{x}}(\mathbf{z})\, \mathrm{d}\mathbb{P}_{\mathbb{X}}(\mathbf{z}) \qquad \text{with} \tag{10}$$

$$\begin{aligned}\mathrm{EFF}_{\mathbf{x}}(\mathbf{z}) = (m_n(\mathbf{z}) - T)\left[2\,\phi\left(\frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \phi\left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \phi\left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right)\right] \\ - \sigma_n(\mathbf{z})\left[2\,\varphi\left(\frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \varphi\left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \varphi\left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right)\right] \\ + \varepsilon(\mathbf{z})\left[\phi\left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \phi\left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right)\right]\end{aligned} \tag{11}$$

φ and ϕ respectively pdf and cdf of $\mathcal{N}(0,1)$, $T^{\pm} := T \pm \varepsilon(\mathbf{z})$ and $\varepsilon(\mathbf{z}) := \kappa\sigma_{n+1}(\mathbf{z})$.

Numerical performances

Test function

- Branin-rescaled function with $T = 10$

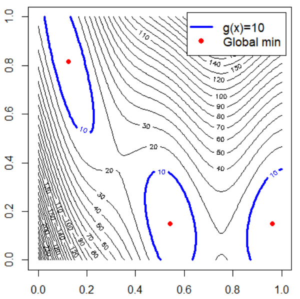

Figure 3: Representation of the Branin2d-rescaled function on $[0, 1]^2$.

Performance comparison measure

- $\mathbb{P}_{\mathbb{X}}(\hat{\Gamma}_n \Delta \Gamma^\star)$ with $\hat{\Gamma}_n$ estimator of the true excursion set $\Gamma^\star$ after n obs.

Performance comparison measure

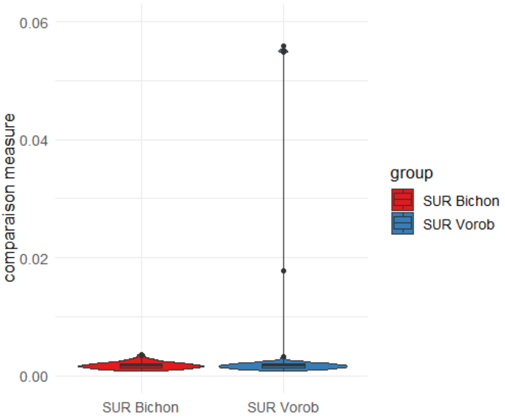

Figure 4: Violin plots of the performance comparaison measure after 20 iterations, in the case of the inversion of the Branin-rescaled function ($d = 2$) with $T = 10$, for 100 different initial DoE of size 10 and type LHS Maximin.

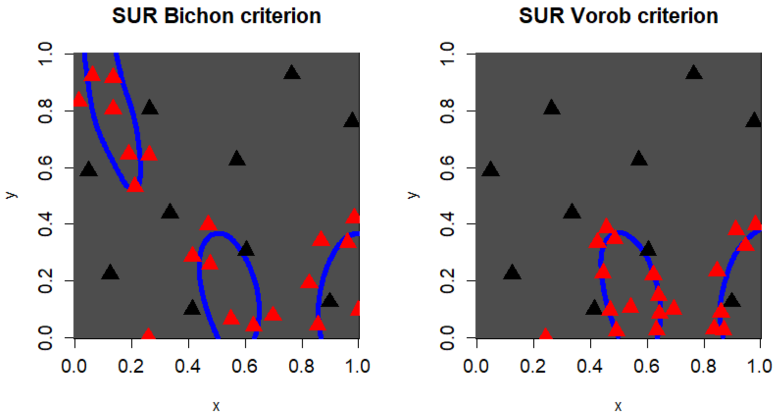

Figure 5: Representation of the $\hat{\Gamma}$ estimators after 20 iterations, in the case of the inversion of the Branin-rescaled function $(d = 2)$ with $T = 10$, for a particular initial DoE where SUR Bichon outperforms on SUR Vorob'ev.

Conclusion

Summary

- SUR adaptation of the Bichon criterion for inversion
  - Simpler to implement than SUR Vorob'ev criterion
  - More robust than SUR Vorob'ev criterion

Next objectives :

- Complete the numerical tests of the inversion based on SUR Bichon criterion (more complex test cases in dimension > 2)
- Add uncertain (functional) variables $(g(\mathbf{x}) := \mathbb{E}_{\mathbf{V}}[f(\mathbf{x}, \mathbf{V})])$
- Generalize the work of Reda El Amri's thesis (*El Amri* [2019]) to probability type constraint instead of expectation

Thank you for your attention

Some references:

El Amri R. [2019]. Analyse d'incertitudes et de robustesse pour les modèles à entrées et sorties fonctionnelles.

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Appendix: Vorob'ev Theory and SUR Vorob'ev criterion

Vorob'ev Theory

- $\Gamma := \{\mathbf{x} \in \mathbb{X}, \xi(\mathbf{x}) \leq T\}$
- Vorob'ev Quantiles: $Q_\alpha := \{\mathbf{x} \in \mathbb{X},\, \mathbb{P}(\mathbf{x} \in \Gamma) \geq \alpha\},\ \forall\, \alpha \in [0,1]$
- Vorob'ev Expectation: $Q_{\alpha^\star}$ such as:

$$\forall \alpha > \alpha^\star,\ \mathbb{P}_{\mathbb{X}}(Q_\alpha) < \mathbb{E}\big[\mathbb{P}_{\mathbb{X}}(\Gamma)\big] \leq \mathbb{P}_{\mathbb{X}}(Q_{\alpha^\star}) \tag{12}$$

- Vorob'ev Deviation: $\mathbb{E}\big[\mathbb{P}_{\mathbb{X}}(\Gamma \Delta Q_{\alpha^\star})\big]$

SUR Vorob'ev criterion

- SUR strategy with uncertainty measure := Vorob'ev Deviation conditionnally to $\mathscr{E}_n$.