ETICS 2021 Presentation

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A SUR version of the Bichon criterion for excursion set estimation

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Introduction: inversion framework

Excursion set to estimate:

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

with

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

Essential criterion to Γ^* estimation:

- Limit the number of g's expensive simulations

Application: floating wind turbine calibration

- Estimation of fitting parameters to limit the error on site measurement (accelerations)

Table of contents:

Reminders on surrogate models and GP regression

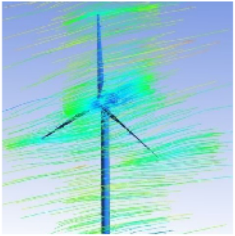
Surrogate models

Surrogate models

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

Gaussian Process Regression (GPR)

- Hypothesis: g is a realization of a gaussian process (GP)



Sequential construction of a DoE by GPR

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

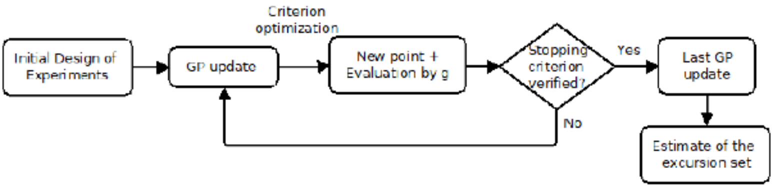


Figure 1: Functional diagram of the DoE sequential construction, by GPR.

Criterion choice

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

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
- $g(\mathscr{X}_n) := (g(\mathbf{x}_1), ..., g(\mathbf{x}_n))$: evaluations on the sequential DoE
- $\mathscr{F}_n$: σ-algebra generated by observations $(\mathscr{X}_n, g(\mathscr{X}_n))$
- $m_n(\mathbf{x}) := \mathbb{E}\left[\xi(\mathbf{x}) \middle| \mathscr{F}_n\right]$: prediction mean
- $k_n(\mathbf{x}, \mathbf{x}') := \mathrm{Cov}\left[\xi(\mathbf{x}), \xi(\mathbf{x}') \middle| \mathscr{F}_n\right]$
- $\sigma_n(\mathbf{x}) := \sqrt{k_n(\mathbf{x}, \mathbf{x})}$: prediction standard deviation
- $\mathbb{P}_{\mathbb{X}}$ a finite measure given on $\mathbb{X}$ (e.g. Lebesgue measure)

Bichon criterion (EFF)

Definition (*Bichon* [2008])

Feasibility Function

$$\begin{aligned} \mathrm{FF}(\mathbf{x}) &:= \varepsilon(\mathbf{x}) - \min\left\{|T - \xi(\mathbf{x})|, \varepsilon(\mathbf{x})\right\} \\ &= \left(\varepsilon(\mathbf{x}) - |T - \xi(\mathbf{x})|\right)^+ \\ &= \begin{cases} \varepsilon(\mathbf{x}) - |T - \xi(\mathbf{x})| & \text{if } \xi(\mathbf{x}) \in \left[T - \varepsilon(\mathbf{x}), T + \varepsilon(\mathbf{x})\right] \\ 0 & \text{otherwise} \end{cases} \end{aligned} \quad (2)$$

with $\varepsilon(\mathbf{x}) := \alpha\sigma_n(\mathbf{x})$

Expected Feasibility Function

$$\mathrm{EFF}(\mathbf{x}) := \mathbb{E}\left[\left(\epsilon(\mathbf{x}) - |T - \xi(\mathbf{x})|\right)^+ \mid \mathscr{F}_n\right] \quad (3)$$

Enrichment of the DoE

$$\mathbf{x}_{n+1} := \underset{\mathbf{x}\in\mathbb{X}}{\operatorname{argmax}}\, \mathrm{EFF}(\mathbf{x}) \quad (4)$$

Interpretation

Interpretation of Feasibility Function

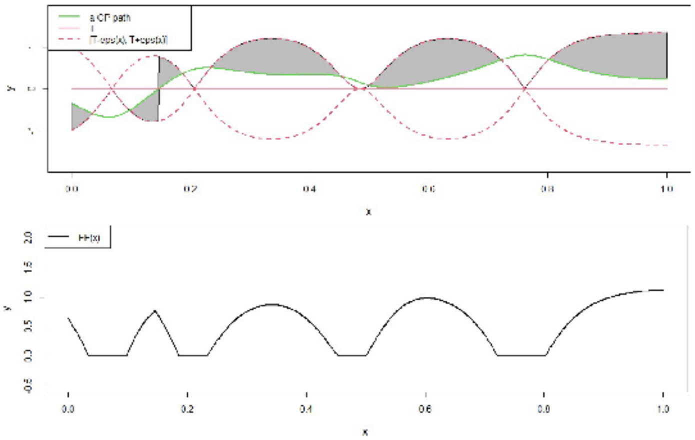


Figure 2: Representation of Feasibility Function for an example of a GP path.

SUR Strategies (*Bect* [2012])

Idea

- An adaptive strategy class
- Anticipate the impact of adding the next evaluation(s)
- Complex formalism resulting from k-step lookahead strategies
- Possible enrichment by q-batch

Simplified formulation with $q = 1$ (and $k = 1$)

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

with

- H_{n+1} uncertainty measure $\mathscr{F}_{n+1}$-measurable

Example (*Chevalier* [2013])

- SUR Vorob'ev criterion:

$$H^V_{n+1} := \mathbb{E}\left[\mathbb{P}_{\mathbb{X}}\left(\Gamma \Delta Q_{n+1,\alpha^*_{n+1}}\right) \,\middle|\, \mathscr{F}_{n+1}\right] \quad (6)$$

with $Q_{n+1,\alpha^*_{n-1}}$ Vorob'ev expectation and $\Gamma := \{\mathrm{x} \in \mathbb{X}, \xi(\mathrm{x}) \leq T\}$ (see Appendix)

Major problem of SUR strategies

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

SUR Bichon criterion

Theoretical aspects

Idea

- Propose a SUR version of the Bichon criterion
- uncertainty measure: integral of Bichon criterion generated by $\mathscr{F}_{n+1}$ according to $\mathbb{P}_{\mathbb{X}}$ measure

Simplified formulation with $q = 1$

$$H^{B}_{n+1} := \int_{\mathbb{X}} \mathbb{E}\left[\left(\alpha\sigma_{n+1}(\mathbf{y}) - |T - \xi(\mathbf{y})|\right)^{+} \,\middle|\, \mathscr{F}_{n+1}\right] \mathrm{d}\mathbb{P}_{\mathbb{X}}(\mathbf{y}) \tag{7}$$

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

Simplifications

$$\mathbf{x}_{n+1} \in \arg\min_{\mathbf{x}\in\mathbb{X}} \mathscr{J}_n(\mathbf{x}) \tag{8}$$

with

$$\begin{aligned}
\mathscr{J}_n(\mathbf{x}) &:= \mathbb{E}\left[\int_{\mathbb{X}} \mathbb{E}\left[\left(\alpha\sigma_{n+1}(\mathbf{y}) - |T-\xi(\mathbf{y})|\right)^+ \,\middle|\, \mathscr{F}_{n-1}\right] \mathrm{d}\mathbb{P}_{\mathbb{X}}(\mathbf{y}) \,\middle|\, \xi(\mathbf{x}), \mathscr{F}_n\right] \\
&\overset{\text{Fubini}}{=} \int_{\mathbb{X}} \mathbb{E}\left[\mathbb{E}\left[\left(\alpha\sigma_{n+1}(\mathbf{y}) - |T-\xi(\mathbf{y})|\right)^- \,\middle|\, \mathscr{F}_{n+1}\right] \,\middle|\, \xi(\mathbf{x}), \mathscr{F}_n\right] \mathrm{d}\mathbb{P}_{\mathbb{X}}(\mathbf{y}) \\
&\overset{*}{=} \int_{\mathbb{X}} \underbrace{\mathbb{E}\left[\left(\alpha\sigma_{n+1}(\mathbf{y}) - |T-\xi(\mathbf{y})|\right)^+ \,\middle|\, \xi(\mathbf{x}), \mathscr{F}_n\right]}_{\mathrm{EFF}_{\mathbf{x}}(\mathbf{y})} \mathrm{d}\mathbb{P}_{\mathbb{X}}(\mathbf{y})
\end{aligned} \tag{9}$$

* by tower property

$\mathrm{EFF}_{\mathbf{x}}(\mathbf{y})$ can be calculated based on $m_n(\mathbf{y})$, $\sigma_n(\mathbf{y})$, T, α and $\sigma_{n+1}(\mathbf{y})$ (see Appendix).

Numerical aspects

Test function

- Branin-rescaled function with T=10 (or T=80)

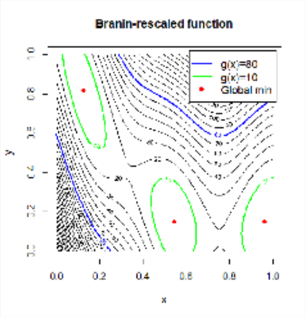


Figure 3: Representation of the Branin2d-rescaled function on $[0,1]^2$.

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

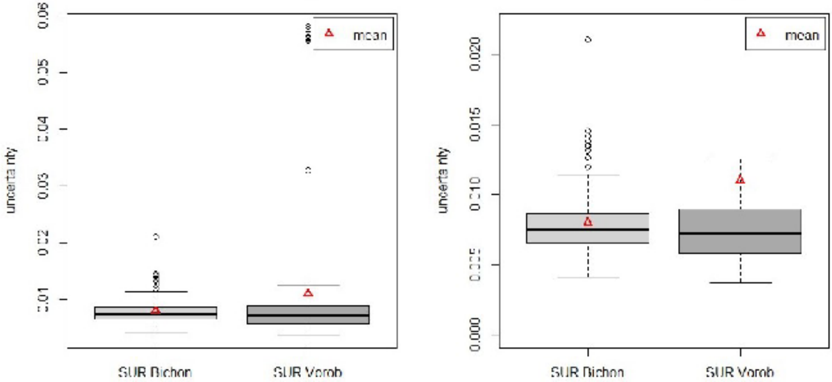


Figure 4: Boxplot (with mean) representation of the performance comparaison measure after 20 iterations, in the case of the inversion of the Branin-rescaled function ($d = 2$) with $T = 10$, for 100 different initial DoE of size 10 and type LHS Maximin.

Conclusion

Summary

- Presenting a SUR version of Bichon criterion
  - Theoretical aspects
  - Numerical aspects

Next objectives :

- Complete the numerical tests of the inversion based on SUR Bichon criterion
- Move to the functional framework ($g(\mathbf{x}) := \mathbb{E}_{\mathbf{V}}[f(\mathbf{x}, \mathbf{V})]$)
- Generalize the work of Reda El Amri's thesis (*El Amri* [2019]) to probability type constraint rather than expectation

Thank you for your attention

Some references:

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- Bect J., Ginsbourger D., Li L., Picheny V., Vazquez E. [2012] Sequential design of computer experiments for the estimation of a probability of failure.
- Chevalier C., Bect J., Ginsbourger D., Vazquez E., Picheny V., et al. [2014] Fast parallel kriging-based stepwise uncertainty reduction with application to the identification of an excursion set.
- Chevalier C., Picheny V., and Ginsbourger D. [2014] Kriginv : An efficient and user-friendly implementation of batch-sequential inversion strategies based on kriging.
- Bichon B. J., and al. [2008] Efficient Global Reliability Analysis for Nonlinear Implicit Performance Functions.
- Pronzato L., Müller W. [2012] Design of computer experiments: space filling and beyond.
- Chevalier C. [2013] Fast uncertainty reduction strategies relying on Gaussian process models.

Appendix: Explicit formula of the SUR Bichon criterion

Property

Noting $T^{\pm} := T \pm \epsilon(\mathbf{y})$ and $\varepsilon(\mathbf{y}) := \alpha\, \sigma_{n+1}(\mathbf{y})$

$$\begin{aligned}\mathrm{EFF}_{\mathbf{x}}(\mathbf{y}) = (m_n(\mathbf{y}) - T)\left[2\,\phi\left(\frac{T - m_n(\mathbf{y})}{\sigma_n(\mathbf{y})}\right) - \phi\left(\frac{T^- - m_n(\mathbf{y})}{\sigma_n(\mathbf{y})}\right) - \phi\left(\frac{T^+ - m_n(\mathbf{y})}{\sigma_n(\mathbf{y})}\right)\right] \\ - \sigma_n(\mathbf{y})\left[2\,\varphi\left(\frac{T - m_n(\mathbf{y})}{\sigma_n(\mathbf{y})}\right) - \varphi\left(\frac{T^- - m_n(\mathbf{y})}{\sigma_n(\mathbf{y})}\right) - \varphi\left(\frac{T^+ - m_n(\mathbf{y})}{\sigma_n(\mathbf{y})}\right)\right] \\ + \epsilon(\mathbf{y})\left[\phi\left(\frac{T^+ - m_n(\mathbf{y})}{\sigma_n(\mathbf{y})}\right) - \phi\left(\frac{T^- - m_n(\mathbf{y})}{\sigma_n(\mathbf{y})}\right)\right]\end{aligned} \tag{10}$$

with φ and ϕ respectively the pdf and cdf of the normal distribution.

This expression can be reinjected in equation (9) to be minimized.

$$\mathscr{J}_n(\mathbf{x}) = \int_{\mathbb{X}} \mathrm{EFF}_{\mathbf{x}}(\mathbf{y})\, \mathrm{d}\mathbb{P}_{\mathbb{X}}(\mathbf{y})$$

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_{α^*} such as:

$$\forall \alpha > \alpha^*, \mathbb{P}_{\mathbb{X}}(Q_\alpha) < \mathbb{E}\left[\mathbb{P}_{\mathbb{X}}(\Gamma)\right] \leq \mathbb{P}_{\mathbb{X}}(Q_{\alpha^*}) \tag{11}$$

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

SUR Vorob'ev criterion

- SUR Strategy with: uncertainty = Vorob'ev Deviation conditionnally to $\mathscr{F}_{n-1}$.

Appendix: SUR criterion performance: outliers

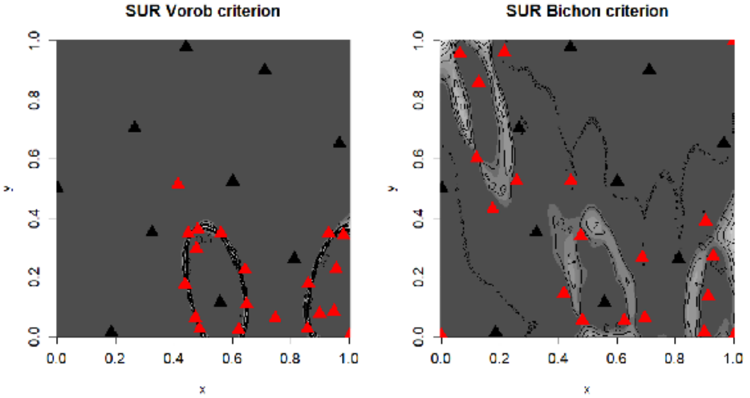

Figure 5: Representation of the Vorob'ev deviation (resp. Bichon uncertainty) for the SUR Vorob'ev (resp. SUR Bichon) criterion, in the case of the inversion of the Branin-rescaled ($d = 2$) function with $T = 10$ and for a particular initial DoE of size 10 and type LHS Maximin, after an enrichment of 20 points.