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Métamodèles pour l'estimation de bornes de défaillance par des inégalités de concentration de mesures optimales

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DTIS/DAAA Métamodèles pour la conception, 22 mars 2023

Uncertainty quantification vs. robust certification

- "Les industriels se plaignent de ne pas voir assez de propagation d'incertitudes dans le PSS" (AM 21/07/2015);
- FP7 UMRIDA (2013-2016, PI C. Hirsch):
  1. "Address major research challenges in both UQ and RDM to develop new methods able to **handle large numbers of simultaneous uncertainties** [...];"
  2. "Apply the UQ and RDM methods to representative industrial configurations. [...] A new generation of database, formed by industrial challenges, provided by the industrial partners, **with prescribed uncertainties**, is established."
- Optimization in terms of a **mean**, **nominal**, or **extreme** performance ("hero calculation").
- But the **probability** of deviating from that nominal performance may be non negligible!

Outline

The UQ problem in a robust certification context

- Uncertainty Quantification (UQ) usually refers to the quantitative characterization and reduction of uncertainties in physical processes (computational or real-world problems).
- Certification is defined here as the process of guaranteeing that the probability $\mathbb{P}$ of exceeding a given threshold a is below an acceptable tolerance ϵ:

$$\boxed{\mathbb{P}_{\boldsymbol{X}\sim\mu^\dagger}[F(\boldsymbol{X}) \geq a] = \mathbb{E}_{\boldsymbol{X}\sim\mu^\dagger}\{\mathbb{1}(F(\boldsymbol{X}) \geq a)\} \leq \epsilon},$$

  where F is the performance function and $\boldsymbol{X}$ are the variable input parameters following the distribution $\mu^\dagger$;
- $\mathbb{P}_{\boldsymbol{X}\sim\mu^\dagger}[F(\boldsymbol{X}) \geq a]$ will be called "probability of failure."
- **Robust certification**: finding bounds on the "probability of failure."

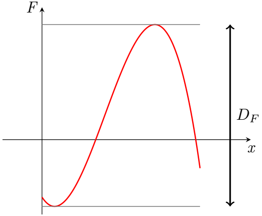
Concentration-of-measure (CoM)

- A real function $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ oscillating about its mean $\mathbb{E}\{F(\boldsymbol{X})\}$ without *a priori* knowledge of the PDFs of the random inputs $\boldsymbol{X} = (X_1, \dots X_d)^\mathsf{T} : \Omega \to \mathcal{X} = \mathcal{X}_1 \times \cdots \times \mathcal{X}_d$.
- Assuming that the latter are independent, the following McDiarmid's inequality holds for all $a > 0$:

$$\mathbb{P}\left[|F(\boldsymbol{X}) - \mathbb{E}\{F(\boldsymbol{X})\}| \geq a\right] \leq \exp\left(-2\frac{a^2}{D_F^2}\right),$$

where $D_F = \left(\sum_{j=1}^d \mathrm{Osc}_j(F)^2\right)^{\frac{1}{2}}$ is the verification diameter of the function F, and for $1 \leq j \leq d$:

$$\mathrm{Osc}_j(F) = \sup_{\boldsymbol{x}\in\mathcal{X}} \sup_{x_j'\in\mathcal{X}_j} \left|F(x_1, \dots x_{j-1}, x_j, x_{j+1}, \dots x_d) - F(x_1, \dots x_{j-1}, x_j', x_{j+1}, \dots x_d)\right| .$$



S. Boucheron, G. Lugosi, P. Massart. *Concentration Inequalities*. Oxford University Press, Oxford (2013)
M. Ledoux. *The Concentration-of-Measure Phenomenon*. American Mathematical Society, Providence RI (2001)
https://terrytao.wordpress.com/2010/01/03/254a-notes-1-concentration-of-measure/

Examples

- Let $F(\boldsymbol{X}) = \frac{1}{d}\sum_{j=1}^{d} X_j$ and $\mathcal{X}_j = [a_j, b_j]$. Then $\mathrm{Osc}_j(F) = \frac{1}{d}(b_j - a_j)$, and the following Hoeffding's inequality holds for all $a > 0$:

$$\mathbb{P}\left[|F(\boldsymbol{X}) - \mathbb{E}\{F(\boldsymbol{X})\}| \geq a\right] \leq \exp\left(\frac{-2a^2d^2}{\sum_{j=1}^{d}(b_j - a_j)^2}\right) .$$

  Thus if $b_j - a_j = \Delta$ for all inputs, one has:

$$\mathbb{P}\left[|F(\boldsymbol{X}) - \mathbb{E}\{F(\boldsymbol{X})\}| \geq a\right] \leq \exp\left(-2d\frac{a^2}{\Delta^2}\right) ;$$

  the higher d is, the less $F(\boldsymbol{X})$ deviates from its mean $\mathbb{E}\{F(\boldsymbol{X})\}$.
- CoM phenomenon: functions over high-dimensional spaces with small local oscillations in each variable are almost constant (Paul Levy 1951).

Examples

- Markov's inequality for a non-negative r.v. X s.t. $\mathbb{E}\{X\} < +\infty$:

$$\mathbb{P}\left[X \geq a\right] \leq \frac{\mathbb{E}\{X\}}{a} \, .$$

- Chebyshev's inequality for $x \mapsto F(x)$ monotonous, non-decreasing:

$$\mathbb{P}\left[X \geq a\right] \leq \frac{\mathbb{E}\{F(X)\}}{F(a)} \, .$$

Application to certification

- **Performance measure**: assume $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ is a performance measure of the system under consideration, such as a limit stress in structural design for which $\boldsymbol{X}$ are d varying geometrical parameters, physical parameters, operational conditions, numerical error sources, *etc.*
- Performance is formulated as the constraint $\{F(\boldsymbol{X}) \leq a\}$, where a: target threshold for the operation of the system.
- Then McDiarmid's inequality yields:

$$\mathbb{P}\left[F(\boldsymbol{X}) \geq a\right] \leq \exp\left(-2\frac{(a-\mathbb{E}\{F(\boldsymbol{X})\})_+^2}{D_F^2}\right) \leq \epsilon\,,$$

  where $x_+ := \max(0, x)$ (this thresholding stems from the fact that if the mean performance is $\mathbb{E}\{F(\boldsymbol{X})\} \geq a$ then very little chance remains to certify the system).
- **Quantification of margins and uncertainties**:
  - $(a - \mathbb{E}\{F(\boldsymbol{X})\})_+$ is the margin M;
  - D_F is the uncertainty measure U;
  - $\mathrm{CF} = \frac{M}{U}$ is then the confidence factor.

  Therefore $\mathbb{P}[F(\boldsymbol{X}) \geq a] \leq \epsilon$ provided that the confidence factor is $\mathrm{CF} > \sqrt{\ln\sqrt{\frac{1}{\epsilon}}}$.

L. J. Lucas, H. Owhadi, M. Ortiz. *Comput. Methods Appl. Mech. Engrg.* **197**(51-52), 4591-4609 (2008)

Application to certification

- **Performance measures**: the analysis extends to multiple performance measures, formulated as *e.g.* the constraints $\{F_1(\boldsymbol{X}) \leq a_1\} \cap \{F_2(\boldsymbol{X}) \geq a_2\}$.
- Then McDiarmid's inequality yields:

$$\begin{aligned}\mathbb{P}\left[\{F_1(\boldsymbol{X}) \geq a_1\} \cap \{F_2(\boldsymbol{X}) \leq a_2\}\right] \\ \leq \exp\left(-2\frac{(a_1 - \mathbb{E}\{F_1(\boldsymbol{X})\})_+^2}{D_1^2}\right) + \exp\left(-2\frac{(\mathbb{E}\{F_2(\boldsymbol{X})\} - a_2)_+^2}{D_2^2}\right).\end{aligned}$$

L. J. Lucas, H. Owhadi, M. Ortiz. *Comput. Methods Appl. Mech. Engrg.* **197**(51-52), 4591-4609 (2008)

Model-based certification

- The goal is to achieve rigorous certification with a maximum use of modeling and simulation and a minimum use of testing.
- Assume a (low-fidelity) model $\boldsymbol{X} \mapsto G(\boldsymbol{X})$ is used to assess the (high-fidelity) system response function, or performance $\boldsymbol{X} \mapsto F(\boldsymbol{X})$.
- Applying once again McDiarmid's inequality to F yields:

$$\begin{aligned}\mathbb{P}\left[F(\boldsymbol{X}) \geq a\right] &\leq \exp\left(-2\frac{(a-\mathbb{E}\{F(\boldsymbol{X})\})_+^2}{D_F^2}\right)\\ &\leq \exp\left(-2\frac{(a-\mathbb{E}\{F(\boldsymbol{X})\})_+^2}{(D_G+D_{F-G})^2}\right),\end{aligned}$$

owing to the triangular inequality $D_F \leq D_G + D_{F-G}$.

Model-based certification

- The mean performance $\mathbb{E}\{F(\boldsymbol{X})\}$ is assessed from legacy data, testing, or MDO for example;[a]
- D_G is the predicted model diameter, *i.e.* a measure of the system uncertainty obtained by exerting the model without any testing;
- D_{F-G} is the model-error diameter, *i.e.* a quantitative measure of the model fidelity, or the discrepancy between model predictions and legacy data/experimental observations.
- One expects $D_{F-G} \lll D_F$ and $D_{F-G} \lll D_G$ for high-fidelity models, whence the number of tests required to compute D_{F-G} is minimized because (iterative) global optimization algorithms may converge rapidly.

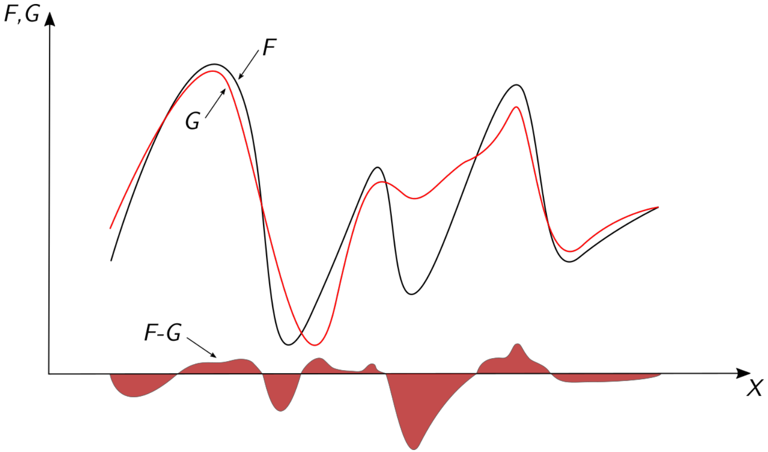
[a] Empirical mean $\underline{F} = \frac{1}{m}\sum_{j=1}^{m} F(\boldsymbol{X}_j)$ such that $D_{\underline{F}}^2 = \frac{1}{m}D_F^2$ and:

$$\mathbb{P}\left[|\underline{F} - \mathbb{E}\{F(\boldsymbol{X})\}| \geq \alpha\right] \leq \exp\left(-2\frac{\alpha^2}{D_{\underline{F}}^2}\right) = \epsilon' \,.$$

Then the margin is reduced by α: $M' = (a - \alpha - \underline{F})_+$ where $\alpha = U\sqrt{\frac{1}{m}\ln\sqrt{\frac{1}{\epsilon'}}}$, but the uncertainty measure $U = D_F$ is unchanged; with probability $1-\epsilon'$:

$$\mathbb{P}\left[F(\boldsymbol{X}) \geq a\right] \leq \exp\left(-2\frac{M'^2}{U^2}\right) \,.$$

Model-based certification



Outline

Optimal Uncertainty Quantification

- One wants to certify $\mathbb{P}_{\boldsymbol{X}\sim\mu^\dagger}\left[F(\boldsymbol{X}) \geq a\right] \leq \epsilon$ **BUT** so far:
  1. F and $\mu^\dagger$ are not known exactly!!!
  2. One only knows $(F, \mu^\dagger) \in \mathcal{A}$ where:

$$\mathcal{A} \subset \left\{ (f, \mu) \;\middle|\; \begin{array}{l} f : \mathcal{X} \to \mathbb{R} \\ \mu \in \mathcal{P}(\mathcal{X}) \end{array} \right\} .$$

"When in doubt, assume the worst!"

- Alternatively one wants to compute optimal bounds:

$$\mathcal{U}[\mathcal{A}] = \sup_{(f,\mu)\in\mathcal{A}} \mu[f(\boldsymbol{X}) \geq a] ,$$

$$\mathcal{L}[\mathcal{A}] = \inf_{(f,\mu)\in\mathcal{A}} \mu[f(\boldsymbol{X}) \geq a] ,$$

such that $\mathcal{L}[\mathcal{A}] \leq \mathbb{P}_{\boldsymbol{X}\sim\mu^\dagger}\left[F(\boldsymbol{X}) \geq a\right] \leq \mathcal{U}[\mathcal{A}]$ and therefore:

- If $\mathcal{U}[\mathcal{A}] \leq \epsilon$: the system is safe even in worst case;
- If $\mathcal{L}[\mathcal{A}] > \epsilon$: the system is unsafe even in best case;
- If $\mathcal{L}[\mathcal{A}] \leq \epsilon < \mathcal{U}[\mathcal{A}]$: one cannot decide.

Optimal Uncertainty Quantification

- **Reduction theorem**: let

$$\mathcal{A} = \left\{ (f,\mu) \;\middle|\; \begin{array}{c} f : \mathcal{X}_1 \times \cdots \times \mathcal{X}_d \to \mathbb{R} \\ \mu = \mu_1 \otimes \cdots \otimes \mu_d \\ \mathcal{C}_j(f,\mu) \leq 0\,,\; 1 \leq j \leq n_0 \\ \mathcal{C}_{j_k}(f,\mu_k) \leq 0\,,\; 1 \leq j_k \leq n_k \end{array} \right\} ;$$

  then $\mathcal{U}[\mathcal{A}] = \mathcal{U}[\mathcal{A}_\Delta]$ where:

$$\mathcal{A}_\Delta = \left\{ (f,\mu) \in \mathcal{A} \;\middle|\; \begin{array}{c} \mu_k = \displaystyle\sum_{i=0}^{n_0+n_k} \alpha_i \delta_{x_i} \\ \alpha_i \geq 0\,, \sum \alpha_i = 1 \end{array} \right\} .$$

- The solution is constructible: open-source `mystic` optimization framework in Python, `https://pypi.org/project/mystic/`, where $\mathcal{U}[\mathcal{A}_\Delta]$ is computed using *e.g.* Storn-Price's Differential Evolution algorithm.
- This constrained optimization problem can be transformed to an unconstrained problem through canonical moments, as shown by J. Stenger in his PhD thesis (2020).

H. Owhadi *et al.* *SIAM Rev.* **55**(2), 271-345 (2013)
R. Storn, K. Price. *J. Global Optim.* **11**(4), 341-359 (1997)
J. Stenger, F. Gamboa, M. Keller, B. Iooss. *Int. J. Uncertain. Quantif.* **10**(1), 35-53 (2020)
T. J. Sullivan. *Introduction to Uncertainty Quantification.* Springer, Cham (2015)

Optimal Uncertainty Quantification

- **Example** (McDiarmid set): let

$$\mathcal{A}_{\mathrm{McD}} = \left\{ (f,\mu) \;\middle|\; \begin{array}{c} f : \mathcal{X}_1 \times \cdots \times \mathcal{X}_d \to \mathbb{R} \\ \mu = \mu_1 \otimes \cdots \otimes \mu_d \\ \mathbb{E}_\mu\{f(\boldsymbol{X})\} \leq 0 \\ \mathrm{Osc}_j(f) \leq D_j \,,\; 1 \leq j \leq d \end{array} \right\} ;$$

then $a \mapsto \mathcal{U}[\mathcal{A}_{\mathrm{McD}}](a) = \sup_{(f,\mu)\in\mathcal{A}} \mu[f(\boldsymbol{X}) \geq a]$ is given for $d = 2$ by:

$$\mathcal{U}[\mathcal{A}_{\mathrm{McD}}](a) = \begin{cases} 0 & \text{if } D_1 + D_2 \leq a \,, \\ \dfrac{(D_1 + D_2 - a)^2}{4 D_1 D_2} & \text{if } |D_1 - D_2| \leq a \leq D_1 + D_2 \,, \\ 1 - \dfrac{a}{\max(D_1, D_2)} & \text{if } 0 \leq a \leq |D_1 - D_2| \,. \end{cases}$$

The solution is explicit for $d = 3$ as well.

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T. J. Sullivan. *Introduction to Uncertainty Quantification.* Springer, Cham (2015)

Outline

Example #1: Deflection of a cantilever beam

- **Performance function**: $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ is the maximum deflection of the beam (in mm) with $\boldsymbol{X} = (E, R)$, where E is its Young's modulus and R its radius.
- One wants to certify that the probability that $F(\boldsymbol{X})$ exceeds the threshold a remains below the tolerance ϵ, *i.e.* $\mathbb{P}[F(\boldsymbol{X}) \geq a] \leq \epsilon$.

- Scenario 0: The performance function $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ and the probability measure $\mu^\dagger$ are exactly known;

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- One wants to certify that the probability that $F(\boldsymbol{X})$ exceeds the threshold a remains below the tolerance ϵ, *i.e.* $\mathbb{P}[F(\boldsymbol{X}) \geq a] \leq \epsilon$.

- Scenario 1: Let $\mathcal{A}_{\mathrm{McD}}$ be McDiarmid's admissible set

$$\mathcal{A}_{\mathrm{McD}} = \left\{ (f, \mu) \;\middle|\; \begin{array}{c} f : \mathcal{X}_1 \times \mathcal{X}_2 \to \mathbb{R} \\ \mu = \mu_1 \otimes \mu_2 \\ \mathbb{E}_{\boldsymbol{X} \sim \mu}\{f(\boldsymbol{X})\} = \mathrm{U} \\ \mathrm{Osc}_j(f) \leq D_j \, , \; 1 \leq j \leq 2 \end{array} \right\} ;$$

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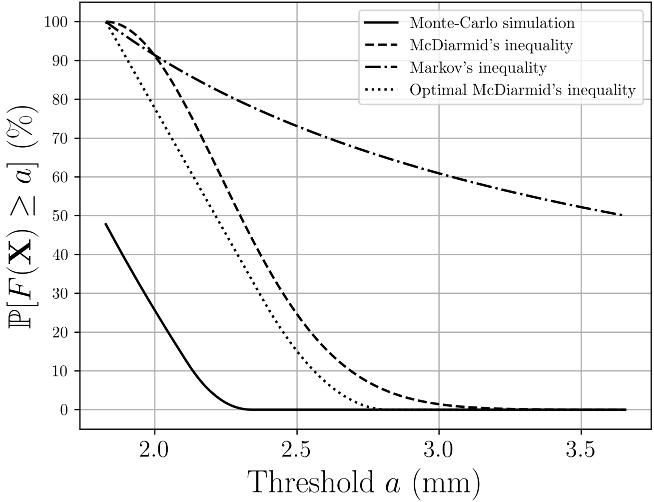
- Scenario 2: Let $\mathcal{A}_F$ be the following admissible set

$$\mathcal{A}_F = \left\{ (F, \mu) \;\middle|\; \begin{array}{c} F : \mathcal{X}_1 \times \mathcal{X}_2 \to \mathbb{R} \text{ is known} \\ \mu = \mu_1 \otimes \mu_2 \\ \mathbb{E}_{\boldsymbol{X}\sim\mu}\{F(\boldsymbol{X})\} = \mathrm{U} \end{array} \right\},$$

where:

$$\begin{array}{lllll} E: & \mathcal{X}_1 = [\underline{E} \pm 5\%]\,\text{GPa} & \underline{E} = 75\,\text{GPa} & D_1 = 0.223\,\text{mm}\,, \\ R: & \mathcal{X}_2 = [\underline{R} \pm 5\%]\,\text{mm} & \underline{R} = 12.5\,\text{mm} & D_2 = 0.722\,\text{mm}\,. \end{array}$$

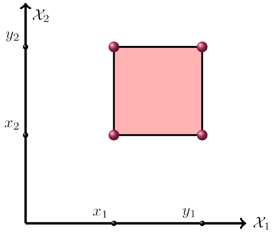
Example #1 – Scenario 1



Example #1 – Scenario 2

- We have from the reduction theorem $\mathcal{U}[\mathcal{A}_F] = \mathcal{U}[\mathcal{A}_\Delta]$ where:

$$\mathcal{A}_\Delta = \left\{ (F,\mu) \in \mathcal{A}_F \;\middle|\; \begin{array}{c} \mu_1 = \alpha_1 \delta_{x_1} + (1-\alpha_1)\delta_{y_1} \\ \mu_2 = \alpha_2 \delta_{x_2} + (1-\alpha_2)\delta_{y_2} \\ \alpha_1, \alpha_2 \geq 0 \\ x_1, y_1 \in \mathcal{X}_1,\; x_2, y_2 \in \mathcal{X}_2 \end{array} \right\} .$$



The marginal measures μ_1 and μ_2 are supported on at most 2 Dirac points. The support of μ consists in at most 4 Dirac support points.

- $\mathcal{U}[\mathcal{A}_\Delta]$ is found using Storn-Price's Differential Evolution algorithm in the `mystic` framework.

R. Storn, K. Price. *J. Global Optim.* **11**(4), 341-359 (1997)

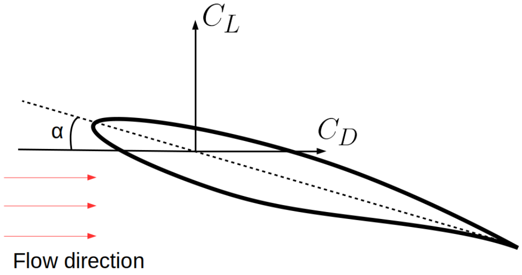
Example #1 – Summary

Threshold		$a = 2.2$ (mm)
Admissible scenario		$\sup_{(f,\mu)\in\mathcal{A}} \mathbb{P}_{\boldsymbol{X}\sim\mu}[f(\boldsymbol{X}) \geq a]$
Scenario 1	McDiarmid's inequality	$\leq 65.1\%$
	$\mathcal{U}[\mathcal{A}_{\mathrm{McD}}]$	$= 51.7\%$
Scenario 2	$\mathcal{U}[\mathcal{A}_F]$	$= 48.7\%$
Scenario 0	$\mathbb{P}[F(\boldsymbol{X}) \geq a]$ (MC over 10^6 samples)	$= 4.4\%$

Upper bounds of the probability of failure with threshold $a = 2.2$ mm for different scenarios.

Example #2: Lift-to-drag ratio for RAE2822

- **Performance measure**: $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ is the lift-to-drag ratio C_L/C_D of a RAE2822 wing profile with $\boldsymbol{X} = (M, \alpha, t)$, where M is the Mach number, α is the angle of attack, and t is some geometrical imperfection.
- One wants to certify that the probability that $F(\boldsymbol{X})$ is lower than a given threshold a remains below the tolerance ϵ, *i.e.* $\mathbb{P}[F(\boldsymbol{X}) \leq a] \leq \epsilon$.
- Computations by ISES, a 2D aerodynamic solver developed by M. Drela and M. B. Giles at MIT.



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- Scenario 0: The performance function $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ and the probability measure $\mu^\dagger$ are exactly known;

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- One wants to certify that the probability that $F(\boldsymbol{X})$ is lower than a given threshold a remains below the tolerance ϵ, *i.e.* $\mathbb{P}[F(\boldsymbol{X}) \leq a] \leq \epsilon$.

- Scenario 1: Let $\mathcal{A}_{\mathrm{McD}}$ be McDiarmid's admissible set

$$\mathcal{A}_{\mathrm{McD}} = \left\{ (f, \mu) \left| \begin{array}{c} f : \mathcal{X}_1 \times \mathcal{X}_2 \times \mathcal{X}_3 \to \mathbb{R} \\ \mu = \mu_1 \otimes \mu_2 \otimes \mu_3 \\ \mathbb{E}_{\boldsymbol{X} \sim \mu}\{f(\boldsymbol{X})\} = \mathrm{L/D} \\ \mathrm{Osc}_j(f) \leq D_j \,, \; j = 1, 2, 3 \end{array} \right. \right\} ;$$

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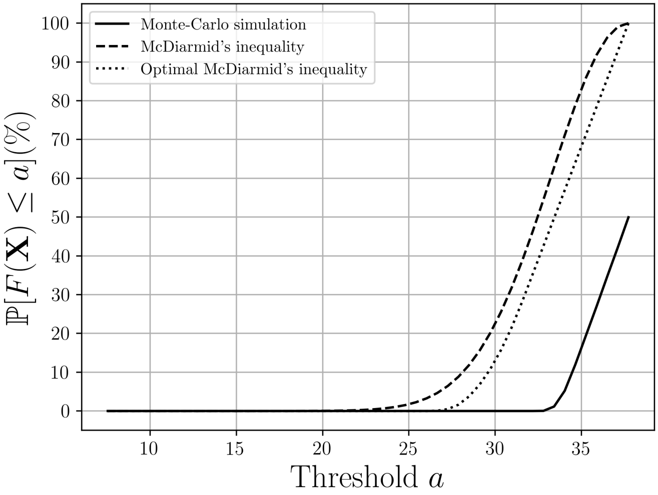
- Scenario 2: Let $\mathcal{A}_F$ be the following admissible set

$$\mathcal{A}_F = \left\{ (F,\mu) \;\middle|\; \begin{array}{c} F : \mathcal{X}_1 \times \mathcal{X}_2 \times \mathcal{X}_3 \to \mathbb{R} \text{ is known} \\ \mu = \mu_1 \otimes \mu_2 \otimes \mu_3 \\ \mathbb{E}_{\boldsymbol{X}\sim\mu}\{F(\boldsymbol{X})\} = \mathrm{L/D} \end{array} \right\},$$

where:

$$\begin{array}{cllll} M: & \mathcal{X}_1 = [\underline{M} \pm 0.05] & \underline{M} = 0.6 & D_1 = 2.435\,, \\ \alpha: & \mathcal{X}_2 = [\underline{\alpha} \pm 0.25^\circ] & \underline{\alpha} = 0.75^\circ & D_2 = 8.579\,, \\ t: & \mathcal{X}_3 = [\underline{t} \pm 5\%] & \underline{t} = 0\% & D_3 = 0.708\,. \end{array}$$

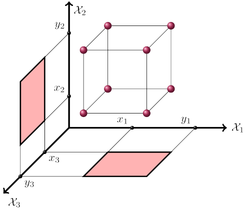
Example #2 – Scenario 1



Example #2 – Scenario 2

- We have from the reduction theorem $\mathcal{U}[\mathcal{A}_F] = \mathcal{U}[\mathcal{A}_\Delta]$ where:

$$\mathcal{A}_\Delta = \left\{ (F,\mu) \in \mathcal{A}_F \;\middle|\; \begin{array}{c} \mu_1 = \alpha_1\delta_{x_1} + (1-\alpha_1)\delta_{y_1} \\ \mu_2 = \alpha_2\delta_{x_2} + (1-\alpha_2)\delta_{y_2} \\ \mu_3 = \alpha_3\delta_{x_3} + (1-\alpha_3)\delta_{y_3} \\ \alpha_1, \alpha_2, \alpha_3 \geq 0 \\ x_1, y_1 \in \mathcal{X}_1,\; x_2, y_2 \in \mathcal{X}_2,\; x_3, y_3 \in \mathcal{X}_3 \end{array} \right\}.$$



The marginal measures μ_1, μ_2 and μ_3 are supported on at most 2 Dirac points. The support of μ consists in at most 8 Dirac support points.

- $\mathcal{U}[\mathcal{A}_\Delta]$ is found using Storn-Price's Differential Evolution algorithm in the `mystic` framework.

R. Storn, K. Price. *J. Global Optim.* **11**(4), 341-359 (1997)

Example #2 – Summary

Threshold		$a = 35$
Admissible scenario		$\sup\limits_{(f,\mu)\in\mathcal{A}} \mathbb{P}_{\boldsymbol{X}\sim\mu}[f(\boldsymbol{X}) \leq a]$
Scenario 1	McDiarmid's inequality	$\leq 83.0\%$
	$\mathcal{U}[\mathcal{A}_{\mathrm{McD}}]$	$= 68.2\%$
Scenario 2	$\mathcal{U}[\mathcal{A}_F]$	$= 65.5\%$
Scenario 0	$\mathbb{P}[F(\boldsymbol{X}) \leq a]$ (MC over 10^5 samples)	$= 16.3\%$

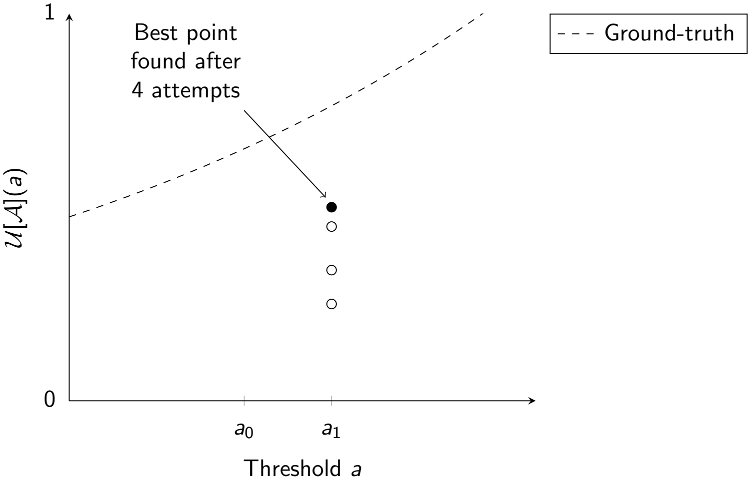
Upper bounds of the probability of failure with threshold $a = 0.35$ for different scenarios.

- $\mathcal{U}[\mathcal{A}_\Delta]$ is computed using *e.g.* Storn-Price's differential evolution algorithm, which can be massively parallelized;
- Even after reduction of the optimization problem this approach remains complex: no optimal solution might ever be found;
- One can use the properties of $a \mapsto \mathcal{U}[\mathcal{A}](a)$ (*e.g.* monotonous) to ensure the validity of the numerical optimal results.

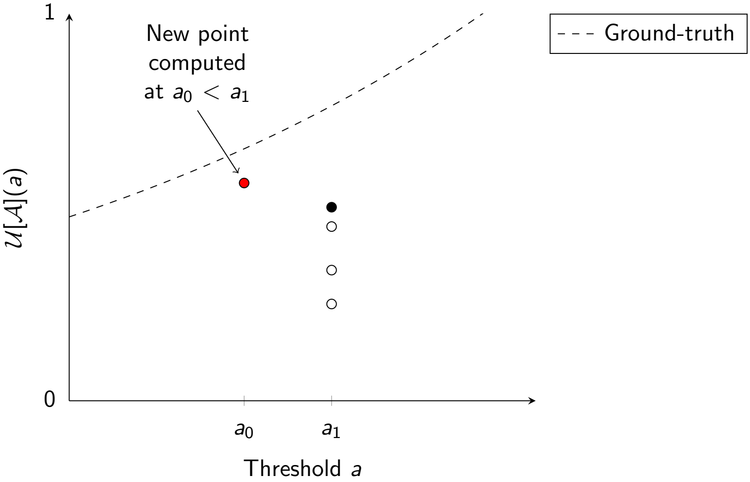
We study the adaptive reconstruction of $a \mapsto \mathcal{U}[\mathcal{A}](a) = \sup_{(f,\mu)\in\mathcal{A}} \mu[f(\boldsymbol{X}) \leq a]$ *when* $a \in [a_0, a_1]$

Outline

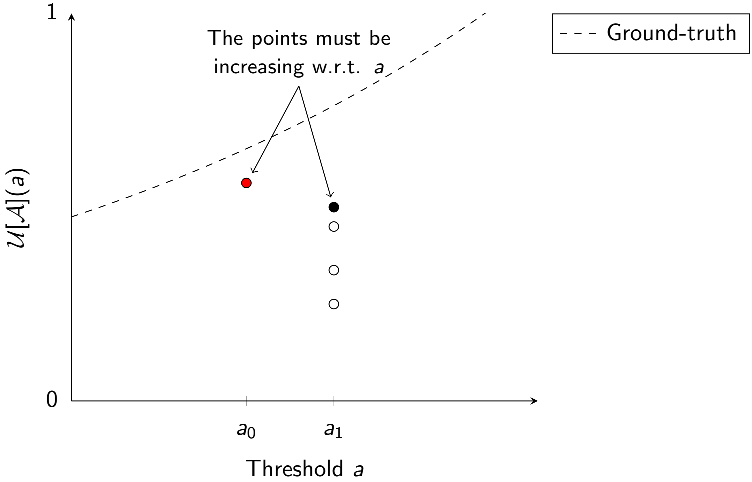
Consistency



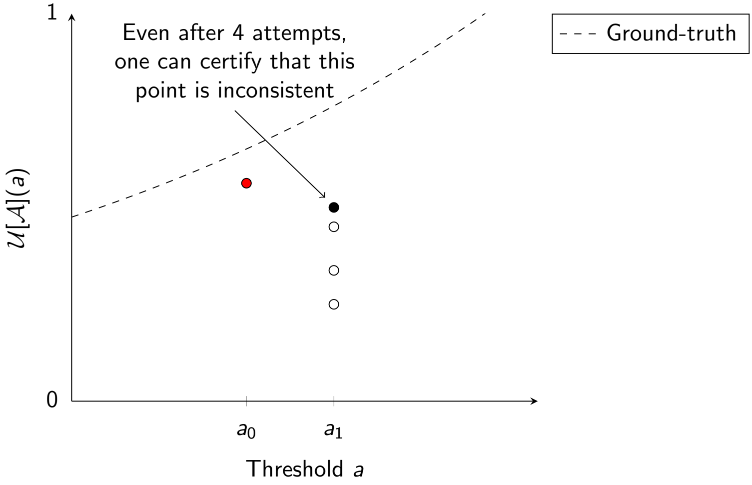
Consistency



Consistency



Consistency

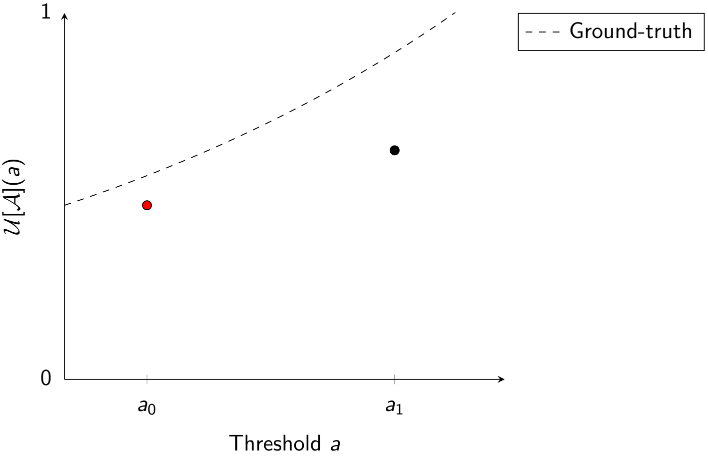


Adaptive reconstruction

- This reasoning can be applied for different properties of the ground-truth function $\mathcal{U}[\mathcal{A}](a)$: increasing, decreasing, convex, *etc*;
- Going further: Reconstruction of the whole ground-truth function over a closed interval $[a_0, a_1]$;
- This can be automated once a metamodel/algorithm $\mathcal{G}(a;q)$ with numerical parameters q is available: L. Bonnet, J.-L. Akian, É. Savin, T. J. Sullivan, *Algorithms* **13**(8),196 (2020).

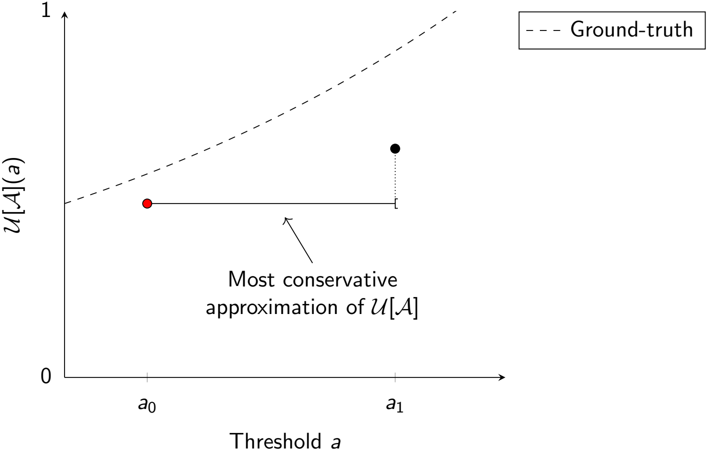
Reconstruction as a piecewise constant function

Reconstruction of the ground-truth function $\mathcal{U}[\mathcal{A}](a)$ on $[a_0, a_1]$ with algorithm $\mathcal{G}(a; q)$



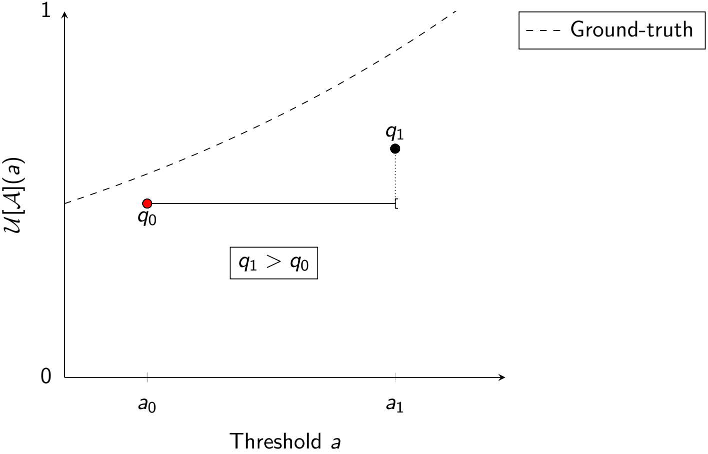
Reconstruction as a piecewise constant function

Reconstruction of the ground-truth function $\mathcal{U}[\mathcal{A}](a)$ on $[a_0, a_1]$ with algorithm $\mathcal{G}(a; q)$



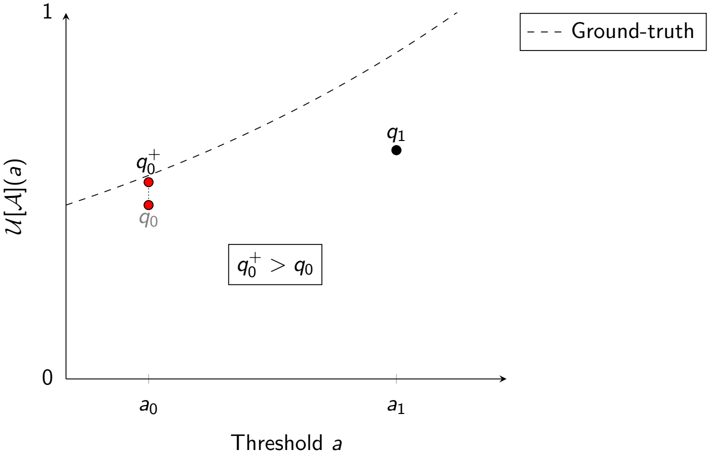
Reconstruction as a piecewise constant function

Reconstruction of the ground-truth function $\mathcal{U}[\mathcal{A}](a)$ on $[a_0, a_1]$ with algorithm $\mathcal{G}(a; q)$



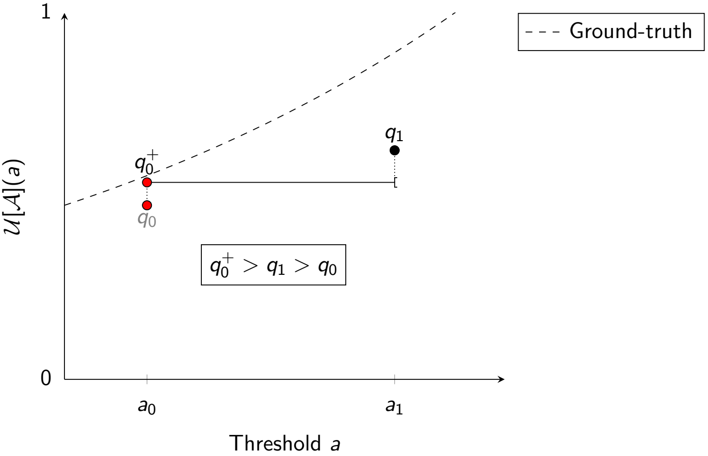
Reconstruction as a piecewise constant function

Reconstruction of the ground-truth function $\mathcal{U}[\mathcal{A}](a)$ on $[a_0, a_1]$ with algorithm $\mathcal{G}(a; q)$



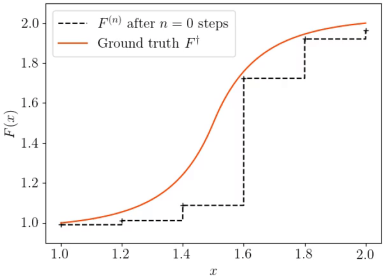
Reconstruction as a piecewise constant function

Reconstruction of the ground-truth function $\mathcal{U}[\mathcal{A}](a)$ on $[a_0, a_1]$ with algorithm $\mathcal{G}(a; q)$



Adaptive reconstruction

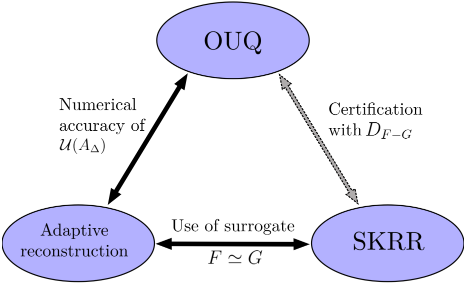
- The choice of redoing a poor-quality evaluation of $\mathcal{U}[\mathcal{A}]$ over adding a new point is controlled by a user-defined parameter $\mathcal{E} > 0$:
  - $\mathcal{E} \gg 1$: Split over redo the worst quality point;
  - $\mathcal{E} \ll 1$: Redo the worst quality point over split.
- The convergence of the algorithm is proved and depend on the smoothness of $\mathcal{U}[\mathcal{A}]$.



Outlook

- Several tens of thousands of function evaluations $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ are typically required to obtain one data point using *e.g.* `mystic` and Storn-Price's algorithm;
- The algorithm is computationally intensive in order to get a new data point;
- Use of a surrogate model $\boldsymbol{X} \mapsto G(\boldsymbol{X})$ is highly desirable. The value obtained through the optimization process will strongly depend on the quality of this surrogate model.

$$\mathcal{U}[\mathcal{A}](a) = \sup_{\mu \in \mathcal{A}} \mu[F(\boldsymbol{X}) \leq a] \simeq \sup_{\mu \in \mathcal{A}} \mu[G(\boldsymbol{X}) \leq a]$$



J.-L. Akian, L. Bonnet, H. Owhadi, É. Savin, *J. Comput. Phys.* **470**, 111595 (2022)