Quantile-based optimization using adaptive Kriging models: Application to car body design

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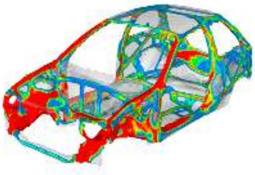
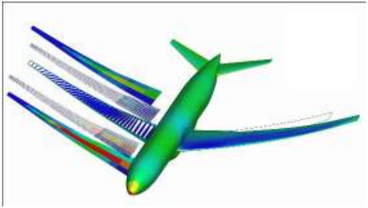
On the necessity of optimization under uncertainties

Structural systems need to be optimized w.r.t. cost constraints





Discrepancy may arise between the designed and actual systems:

- Model error
- Uncertainties
  - in the design parameters (*e.g.* dimensions or material properties)
  - in the environmental conditions (*e.g.* loading)

Accounting for uncertainties

Robust design optimization (RDO)

- Seeks to produce a design immune to input variability
- Puts emphasis on the effects of randomness on the objective function

Reliability-based design optimization (RBDO)

- Trades cost with reliability
- The failure probability P_f gives a measure of the design reliability

$$P_f = \mathbb{P}\left[g\left(\boldsymbol{X}\right) \leq 0\right] = \int_{\mathcal{D}_f = \{\boldsymbol{x} : g(\boldsymbol{x}) \leq 0\}} f_{\boldsymbol{X}}\left(\boldsymbol{x}\right) d\boldsymbol{x}$$

- Estimation of the failure probability
  - Approximation: FORM/SORM
  - Simulation: Monte Carlo or advanced simulation methods
  - Surrogate modeling

Introduction to surrogate modeling

Santner et al. (2003)

- Let us consider a computational model $\mathcal{M}$ which represents the physical behavior of the system:

$$\boldsymbol{X} \in \mathcal{D}_{\boldsymbol{X}} \subset \mathbb{R}^M \mapsto Y = \mathcal{M}\left(\boldsymbol{X}\right) \in \mathbb{R}$$

- The computational model is generally time-consumming and treated as a black-box

- A metamodel $\widehat{\mathcal{M}}$ is a cheap approximation of $\mathcal{M}$ yet with similar statistical properties

- Given an experimental design $\boldsymbol{\mathcal{X}} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_n\}$ and the associated model response $\boldsymbol{\mathcal{Y}} = \{\mathcal{M}\left(\boldsymbol{x}_1\right), \dots, \mathcal{M}\left(\boldsymbol{x}_n\right)\}$:
  - Kriging yields a mean prediction $\mu_{\widehat{\mathcal{M}}}\left(\boldsymbol{x}\right)$ and variance $\sigma^2_{\widehat{\mathcal{M}}}\left(\boldsymbol{x}\right)$
  - The variance gives a local measure of the accuracy of the surrogate, thus allowing for adaptive techniques

Outline

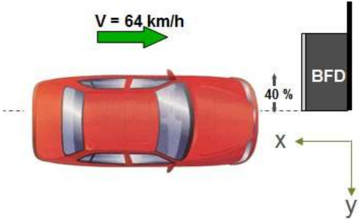
RBDO formulation

Dubourg et al. (2011)

RBDO formulation

$$\boldsymbol{d}^* = \arg\min_{\boldsymbol{d}\in\mathbb{D}} \mathfrak{c}(\boldsymbol{d}) \text{ s.t.: } \begin{cases} \mathfrak{f}_j(\boldsymbol{d}) \leq 0 & \{j = 1, \dots, n_s\} \\ \mathbb{P}\left[\mathfrak{g}_k(\boldsymbol{X}(\boldsymbol{d}), \boldsymbol{Z}) < 0\right] \leq \bar{P}_{f_k} & \{k = 1, \dots, n_h\} \end{cases}$$

- $\boldsymbol{X} \sim f_{\boldsymbol{X}|\boldsymbol{d}}$: Design parameters
- $\boldsymbol{Z} \sim f_{\boldsymbol{Z}}$: Environmental parameters
- $\mathfrak{c}$: Cost function
- $\mathfrak{f}$: Soft constraints
- $\mathfrak{g}$: Hard constraints – $\mathfrak{g}_k(\boldsymbol{X}(\boldsymbol{d}), \boldsymbol{Z}) = \bar{\mathfrak{g}}_k - \mathcal{M}_k(\boldsymbol{X}(\boldsymbol{d}), \boldsymbol{Z})$



RBDO solution

Chateauneuf and Aoues (2008)

Solution of the RBDO problem

- Two-level approach
- Mono-level approach
- Decoupled approach

Application to car body optimization

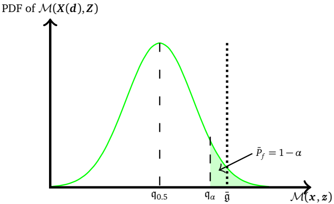
- Structural reliability analysis
  - Approximation methods are inefficient due to the complexity of the limit state
  - The target failure probability is relatively high $(1\% - 10\%)$
- Double-loop optimization
  - Industrial context: The formulation needs to be close to a deterministic design optimization

Solution of the RBDO problem with quantiles as measure of conservatism

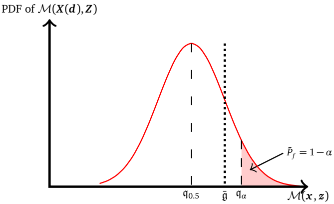
Quantile-based design optimization

- Definition of the quantile

$$Q_\alpha \left(\boldsymbol{d}; \mathcal{M}\left(\boldsymbol{X}\left(\boldsymbol{d}\right), \boldsymbol{Z}\right)\right) = \inf \left\{q \in \mathbb{R} : \mathbb{P}\left[\mathcal{M}\left(\boldsymbol{X}\left(\boldsymbol{d}\right), \boldsymbol{Z}\right) \leq q\right] \geq \alpha\right\}$$



Safe design



Unsafe design

Quantile-based formulation

$$\boldsymbol{d}^* = \arg\min_{\boldsymbol{d}\in\mathbb{D}} \mathfrak{c}\left(\boldsymbol{d}\right) \text{ s.t.: } \begin{cases} \mathfrak{f}_j\left(\boldsymbol{d}\right) \leq 0 & \{j = 1, \ldots, n_s\} \\ Q_{\alpha_k}\left(\boldsymbol{d}; \mathcal{M}\left(\boldsymbol{X}\left(\boldsymbol{d}\right), \boldsymbol{Z}\right)\right) \leq \bar{\mathfrak{g}}_k & \{k = 1, \ldots, n_h\} \end{cases}$$

$\alpha_k = 1 - \bar{P}_{f_k}$ controls the degree of conservatism

Solution of the RBDO problem

Taflanidis (2007), Dubourg (2011)

Monte Carlo simulation in the inner loop

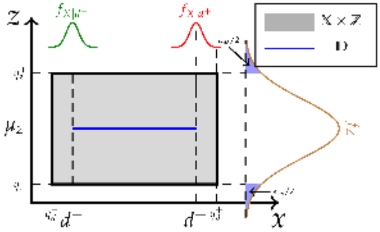
- Quantile computed from the following set of Monte Carlo samples

$$\mathfrak{C}_q = \{(\boldsymbol{x}_j, \boldsymbol{z}_j), j = 1, \dots, N\} \quad \boldsymbol{X} \sim f_{\boldsymbol{X}|\boldsymbol{d}}, \quad \boldsymbol{Z} \sim f_{\boldsymbol{Z}}$$

Construction of the surrogate model

- Build a single global model in the augmented space

A unique space $\mathbb{X} \times \mathbb{Z}$ with high confidence margin such that $\mathbb{P}(\mathfrak{C}_q \subset \mathbb{X} \times \mathbb{Z}) \to 1$



- Adaptive construction

Adaptive enrichment

Echard et al. (2011)

Enrichment principle

- Start with an initial scarce experimental design
- Define a learning function for enrichment
- Enrich the experimental design iteratively so that the Kriging model becomes more accurate in regions of interest

Deviation number

$$U(\boldsymbol{x}) = \frac{\left|\bar{\mathfrak{g}} - \mu_{\widehat{\mathcal{M}}}(\boldsymbol{x})\right|}{\sigma_{\widehat{\mathcal{M}}}(\boldsymbol{x})}$$

- This function is to be minimized with respect to a pre-defined MC set
- U decreases as $\mu_{\widehat{\mathcal{M}}} \to \bar{\mathfrak{g}}$ and/or $\sigma_{\widehat{\mathcal{M}}} \to \infty$
- Stopping criterion: $\min U \geq 2$ (Prob. of misclassification ≈ 0.05)

Too conservative a stopping criterion!

A two-stage of enrichment scheme

Main idea: Couple enrichment to optimization

First stage of enrichment: global

- Identify regions of the space in the vicinity of the limit-state surface
- Reduce the global Kriging epistemic uncertainty in these regions
- Stop when such regions have been discovered without refining too much

Second stage of enrichment: local

- Start the optimization
- Make sure that the computed quantile at each iteration is accurate enough
- If not, locally refine the Kriging model
- Enrichment points are directed toward regions of the space where the objective function is decreasing

First stage of enrichment

Remark: The constraint on the quantile is defined in the design space while the Kriging model is built in the augmented space

A slightly modified enrichment scheme

1. Sample a set of candidates for enrichment: $\mathfrak{C} \in \mathbb{D}$
2. For any $\boldsymbol{d}^{(i)} \in \mathfrak{C}$:
   1. Build the set of MC samples needed to compute the quantile: $\mathfrak{C}_q^{(i)}$
   2. Estimate the quantile $\widehat{\mathfrak{q}}_\alpha \left(\boldsymbol{d}^{(i)} \right)$
   3. Identify the point

   $$(\boldsymbol{x}_\alpha^{(i)}, \boldsymbol{z}_\alpha^{(i)}) = \{ (\boldsymbol{x}, \boldsymbol{z}) \in \mathfrak{C}_q^{(i)} : \widehat{\mathfrak{q}}^\alpha(\boldsymbol{d}^{(i)}) = \mu_{\widehat{\mathcal{M}}}(\boldsymbol{x}, \boldsymbol{z}) \}$$

   4. Compute the modified learning function:

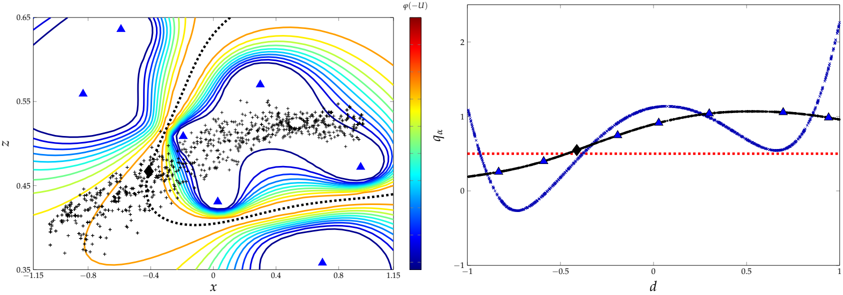
   $$\widetilde{\mathcal{U}} \left(\boldsymbol{d}^{(i)} \right) \equiv U \left(\boldsymbol{x}_\alpha^{(i)}, \boldsymbol{z}_\alpha^{(i)} \right) = \frac{\left| \bar{\mathfrak{g}} - \mu_{\widehat{\mathcal{M}}} \left(\boldsymbol{x}_\alpha^{(i)}, \boldsymbol{z}_\alpha^{(i)} \right) \right|}{\sigma_{\widehat{\mathcal{M}}} \left(\boldsymbol{x}_\alpha^{(i)}, \boldsymbol{z}_\alpha^{(i)} \right)}$$

3. Add K points w.r.t. the modified learning function $\widetilde{\mathcal{U}} \left(\boldsymbol{d} \right)$

Illustration of the global stage of enrichment

Two-dimensional analytical function

- $\mathcal{M}(d,z) = \left(1/3z^4 - 2.1z^2 + 4\right) z^2 + dz + 4d^2\left(d^2 - 1\right)$
- Probabilistic model: $X \sim \mathcal{N}\left(d, 0.05^2\right)$ et $Z \sim \mathcal{N}\left(0.5, 0.05^2\right)$
- $\mathfrak{g}(d,z) = 0.5 - \mathcal{M}(d,z)$ with $\alpha = 0.95$



Second stage of enrichment

- Relax the stopping criterion of the first stage as follows:

$$\eta = \text{Card}(\mathfrak{C}_2)/\text{Card}(\mathfrak{C}) \leq \bar{\eta} \quad \text{where} \quad \mathfrak{C}_2 = \left\{ \boldsymbol{d} \in \mathfrak{C} : \widetilde{\mathcal{U}}\left(\boldsymbol{d}\right) \leq 2 \right\}$$

- Reduce the remaining Kriging epistemic uncertainty during optimization

1. Define the bounds $\widehat{\mathfrak{q}}_\alpha^{\pm}$ as quantiles estimated with $\mu_{\widehat{\mathcal{M}}} \pm 2\sigma_{\widehat{\mathcal{M}}}$:

$$\widehat{\mathfrak{q}}_\alpha^{-}\left(\boldsymbol{d}^{(i)}\right) \leq \widehat{\mathfrak{q}}_\alpha\left(\boldsymbol{d}^{(i)}\right) \leq \widehat{\mathfrak{q}}_\alpha^{+}\left(\boldsymbol{d}^{(i)}\right)$$

2. Compute the following accuracy criterion:

$$\eta_q\left(\boldsymbol{d}^{(i)}\right) = \frac{\widehat{q}_\alpha^{+}\left(\boldsymbol{d}^{(i)}\right) - \widehat{q}_\alpha^{-}\left(\boldsymbol{d}^{(i)}\right)}{\bar{\mathfrak{g}}} \leq \bar{\eta}_q$$

3. If not accurate enough, enrich with the following learning criterion:

$$\mathfrak{U}\left(\boldsymbol{x}, \boldsymbol{z}\right) = \frac{\left|\widehat{\mathfrak{q}}_\alpha\left(\boldsymbol{d}^{(i)}\right) - \mu_{\widehat{\mathcal{M}}}\left(\boldsymbol{x}, \boldsymbol{z}\right)\right|}{\sigma_{\widehat{\mathcal{M}}}\left(\boldsymbol{x}, \boldsymbol{z}\right)}, \qquad \left\{x, z\right\}^T \in \mathfrak{C}_q^{(i)}$$

Presentation of the problem

Deterministic design optimization

- A two-dimensional optimization problem with three non-linear limit state functions:

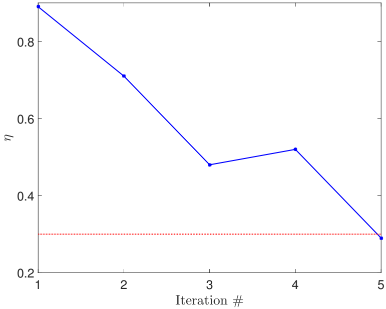
$$\boldsymbol{d}^* = \arg \min_{\boldsymbol{d} \in [0,10]^2} d_1 + d_2 \quad \text{s.t.:} \begin{cases} \frac{d_1^2 d_2}{20} - 1 \leq 0 \\ \frac{(d_1+d_2-5)^2}{30} + \frac{(d_1-d_2-12)^2}{120} - 1 \leq 0 \\ \frac{80}{\left(d_1^2+8d_2+5\right)-1} \leq 0 \end{cases}$$

Reliability-based design optimization

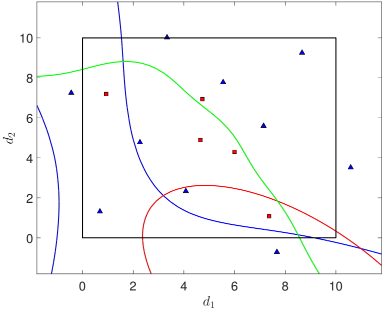
- Probabilistic model: $X_i \sim \mathcal{N}\left(d_i, 0.6^2\right),\ i = \{1,2\}$
- Target failure probability: $\bar{P}_{f_i} = 1.35 \cdot 10^{-3}$ ($\beta_i = 3$).

Solution: First stage of enrichment

- Initial experimental design of size 10
- Threshold for enrichment $\bar{\eta} = 0.30$



Convergence of the enrichment scheme



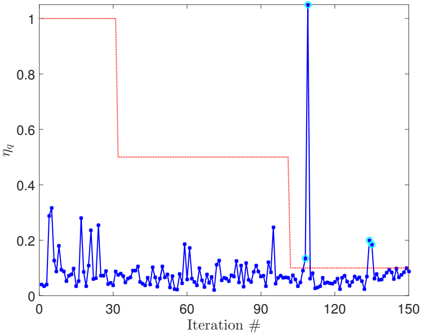
Kriging approximations and updated experimental design

- Convergence in five iterations

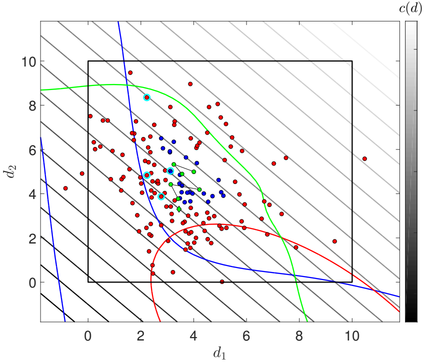
Solution: Second stage of enrichment

Arnold and Hansen (2012)

- Optimization algorithm: Constrained (1+1)-CMA-ES
- Stopping criterion in a simulated-annealing fashion (3 thresholds)



Convergence of the enrichment scheme



Kriging approximations and CMA-ES-sampled points

- Convergence with four enrichments

Benchmark results

- Due to randomness along the process, the results need to be replicated
- Presented result: Median case with respect to 50 random replications

Method	d_1^*	d_2^*	$\mathfrak{c}\left(\boldsymbol{d}^*\right)$	$\mathfrak{g}$-calls
Brute force	3.45	3.30	6.75	$\approx 10^6$
PMA[1]	3.43	3.29	6.72	$1,551$
SORA[2]	3.44	3.29	6.73	151
Single loop[3]	3.43	3.29	6.72	19
RDS[1]	3.44	3.28	6.72	27
Meta-RBDO[4]	3.46	3.27	6.74	$20(20/10/10)$
Quantile-RBDO	3.46	3.30	6.76	14

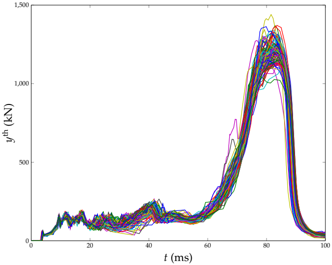
1 As calculated in Shan and Wang (2008)
2 As calculated in Du and Chen (2004)
3 As calculated in Liang et al. (2004)
4 As calculated in Dubourg (2011)

Context of the study

Duddeck (2008)

Multi-disciplinary design optimization problem

- Reduce the weight of a car body structure
- under safety and comfort of use constraints

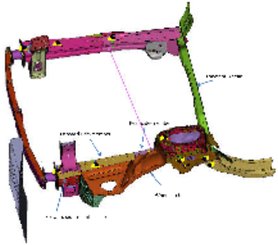


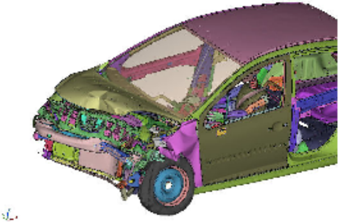
Outputs corresponding to a MC simulation with random input parameters

Focus on the frontal impact alone

- High-dimensional problem
- Time-consuming simulation (up to 24 hours on a HPC infrastructure)
- Highly sensitive to uncertainties

Application to a sidemember subsytem



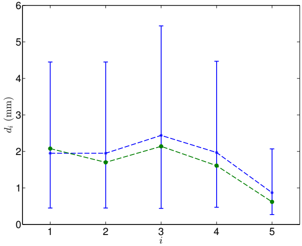


- Five design variables: Metal sheet thicknesses
- Two environmental variables: $V \sim \mathcal{U}(34, 35)$ km/h, $P \sim \mathcal{N}(0, 2)$ mm
- Cost: Weight of selected parts
- Performance functions
  - Wall contact force (kN): $\mathfrak{g}_1 = 170 - \mathcal{M}_1$
  - Sidemember compression (mm): $\mathfrak{g}_2 = 525 - \mathcal{M}_2$
- Target failure probabilities: $\bar{P}_{f_i} = 0.05$ $(\alpha_i = 0.95)$

Solution of the problem

Convergence in only 114 model evaluations

- Initial experimental design: 70 points
- First stage of enrichment: 20 points (2×10)
- Second stage of enrichment: 24 points (8×3)
- Weight saving: 1.31 kg $(13.5\%$ of initial weight$)$



Initial and final thicknesses

Model accuracy estimation in the vicinity of the solution - Computed on a limited MC set of size 100

Criterion	$\mathfrak{g}_1$ (kN)	$\mathfrak{g}_2$ (mm)
Original model $\widehat{\mathfrak{q}}_\alpha^{\text{FE}}$	150.66	527.81
Kriging model $\widehat{\mathfrak{q}}_\alpha^{\text{KRG}}$	148.02	528.04
Error $(\%)$	1.75	0.04

Conclusion

Quantile-based design optimization

- Computed by crude Monte Carlo simulation
- Relatively high target failure probabilities in the applications
- More easily implementable in an industrial context where deterministic design optimization is the cultural reference

Adaptive Kriging-based appproach

- Two stages of enrichment: global then local
- Save computational budget and direct enrichment to regions of high fitness of the cost function

Application in high-dimensional problems

- Successful application in a 23-dimensional problem with 8 constraints
- Accuracy criteria difficult to respect: the approach is based on the idea of Kriging margin shrinking which is hard to achieve in high dimension

Questions ?

Chair of Risk, Safety & Uncertainty Quantification

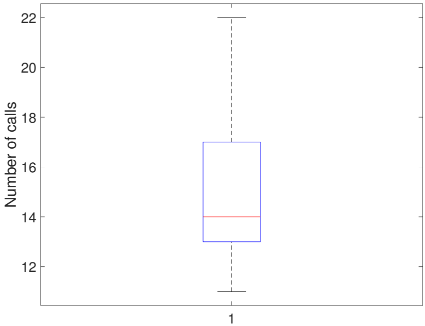
www.rsuq.ethz.ch

The Uncertainty Quantification Laboratory

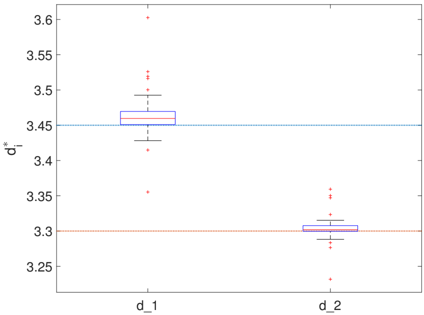
www.uqlab.com

Thank you very much for your attention !

Results with 50 replications for the two-dimensional problem

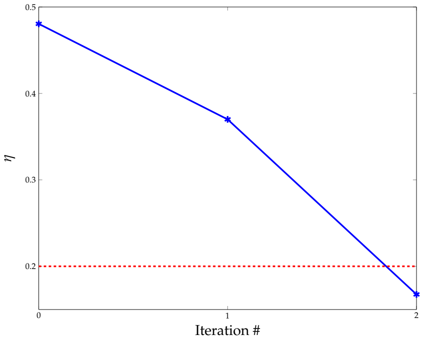


Number of calls to the true model

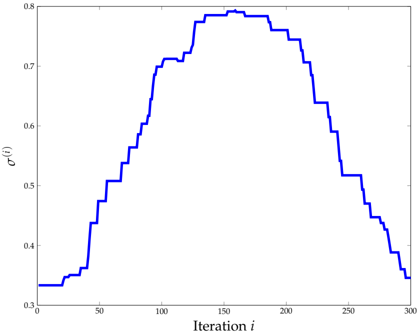


Components of the optimal design

Convergence plots for the sidemember subsystem



Convergence of the first stage of enrichment



Convergence of the CMA-ES algortihm