A mixed intrusive and non-intrusive approximation technique for efficient robust aerodynamic shape design

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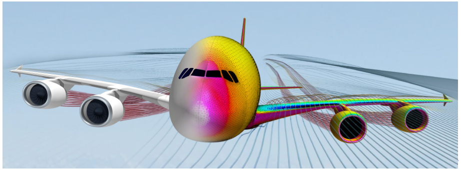

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UTOPIÆ

Uncertainty Treatment and Optimisation in Aerospace Engineering

1. Morales E., Quagliarella D. (2021) **Risk Measures in the Context of Robust and Reliability Based Optimization**, in: Vasile M. (eds), *Optimization Under Uncertainty with Applications to Aerospace Engineering*, Springer, Cham, https://doi.org/10.1007/978-3-030-60166-9_13.
2. Morales, E., Bornaccioni, A., Quagliarella, D. and Tognaccini, R., (2021) **Gradient based empirical cumulative distribution function approximation for robust aerodynamic design', Aerospace Science and Technology**, 2021, 112(5), n. 106630, Elsevier BV, DOI: 10.1016/j.ast.2021.106630.
3. Morales, E., Quagliarella, D. and Tognaccini, R., (2022) **Gaussian Processes for CVaR approximation in Robust Aerodynamic Shape Design**, In: Vasile M., Quagliarella D. (eds), *Advances in Uncertainty Quantification and Optimization Under Uncertainty with Aerospace Applications*, Springer, Cham.

Problem overview

In **Robust Optimisation Problems** the Quantity of Interest (QoI) is a statistical measure.

Increase the number of function evaluations, generally expensive: e.g. CFD evaluations for Aerodynamic Design Problems.

An optimum design less vulnerable to different sources of uncertainty is found.

- Geometrical uncertainties: Manufacturing Tolerances, icing or fatigue of the material.
- Operational uncertainties: Mach number (M) or Angle of Attack (α).
- Model uncertainties (epistemic): lack of knowledge about some physical aspects that the model tries to reproduce.

Therefore, Robust optimization is a very promising field, **BUT** a limit exist: **computationally expensive!**

OBJECTIVE: investigate mixing of intrusive and non-intrusive methods for **risk measure approximation** to **reduce** the **CPU time**.

Problem overview

So, for **robust aerodynamic shape design** fhow can we **reduce** the **computational cost**?

- Speeding up the CFD evaluations.
- Approximating the statistical measure.

→ Surrogate Models (Gaussian Processes) — **non-intrusive approach**.
→ Using the RANS adjoint solution — **intrusive approach**.

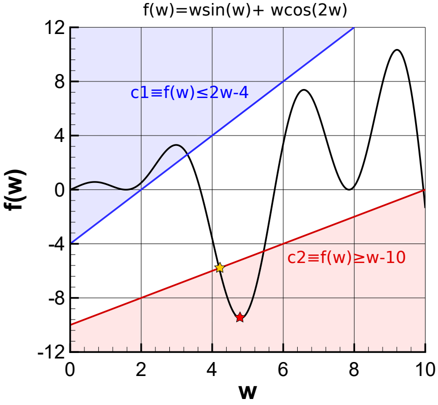
- I order approximation: Gradient calculation.
- II order approximation: Hessian Matrix calculation.

→ **Hybridize intrusive and non-intrusive approaches.**

Deterministic Optimization Problem

Optimization problems are mathematically defined using the minimization formulation.

$$
\begin{cases}
\min\limits_{\mathbf{w}\in S} & f(\mathbf{w}) \\
s.to: & \\
 & c_i(\mathbf{w}) \leq 0 \quad i = 1, \dots, m \\
 & S \subseteq \mathbb{R}^n
\end{cases}
$$



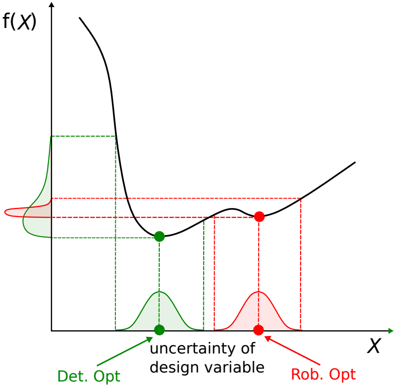
- Objective function: $f(\mathbf{w})$
- Design variables: $\mathbf{w}$
- Constraint functions: $c_i(\mathbf{w})$

Robust Optimization Problem

It offers an **optimal design less vulnerable** to sources of **uncertainty**.

Unknown or **future states** $\rightarrow$ **introduce random variables** X.

$$
\begin{cases}
\min\limits_{\mathbf{w}\in S} & f(\mathbf{w}, X) \\
s.to: & \\
 & c_i(\mathbf{w}, X) \leq 0 \quad i = 1, \ldots, m \\
 & S \subseteq \mathbb{R}^n
\end{cases}
$$



Objective and **constraints** are now **functions**.
Remapped into **real numbers**.

Several approaches are possible, but here **Risk measures** are used.

Stochastic optimisation

It offers an **optimal design less vulnerable** to sources of **uncertainty** (geometrical and operational uncertainties are here considered).

Unknown or **future states** may be taken into account **introducing** (real-valued) **random variables** X.

$$
\begin{cases}
\min\limits_{\mathbf{w}\in S} & f(\mathbf{w}, X) \\
s.to: & \\
 & c_i(\mathbf{w}, X) \leq 0 \quad i = 1, \ldots, m \\
 & S \subseteq \mathbb{R}^n
\end{cases}
$$

Objective and **constraints** are now **functions**. So we have to find a way to **recast** the **problem into** an **optimisation one**.
Several approaches are possible, but here **Risk measures** are used.

Optimisation of Risk Measures

We measure risk introducing a generic risk function $\mathcal{R}(X)$ and agreeing on a level of risk that we consider acceptable, bearing in mind that there will inevitably be adverse events

$$\mathcal{R}(X) \leq C$$

Hence we can write

$$\begin{cases} \min\limits_{\mathbf{z}\in S} & \mathcal{R}_0(f(\mathbf{z}, X)) \\ s.to: & \\ & \mathcal{R}_i(f(\mathbf{z}, X)) \leq 0 \quad i = 1, \dots, m \\ & S \subseteq \mathbb{R}^n \end{cases}$$

- Note that sup can also be considered a risk function *with special requirements for its computation*
- Here, CVaR is used.

Risk Measures for RDO

Which **kind** of **Statistical Measures** can be used? $\rightarrow$ **Risk measures**.

- Classical approach: based on the mean (μ), standard deviation (σ), or combination of both ($\mu + \sigma$).

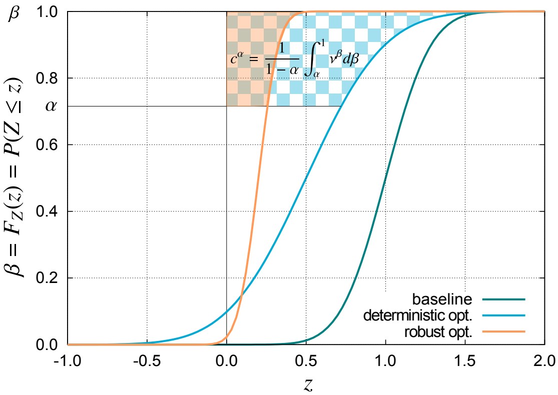
  $\rightarrow$ Penalise all the configurations that are far from the mean value.

  $\rightarrow$ Example: considering we want to minimize the drag coefficient, C_d, these measures will penalize the configurations that will provide a decrease on drag in the same way than the configurations that will increase it.

  $\rightarrow$ But, we only want to penalize configurations that produce an increase on it $\rightarrow$ **Statistical measure** that **works asymmetrically** needed!

Cumulative Distribution Function $\Longrightarrow$ Risk Functions

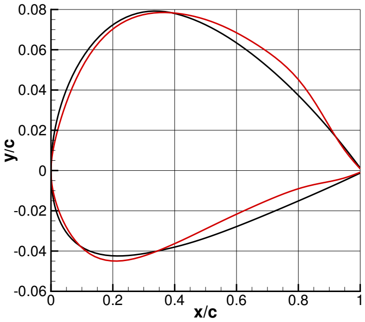
- CDF gives the area under the probability density function from minus infinity to x. $F_Z(z) = \mathrm{P}(Z \le z)$, is the probability that Z takes on a value $\le z$.
- **VaR Minimum value** of z **that makes the CDF** of Z to be **greater than** or **equal to** a **confidence level** α.
  It is the maximum loss that can be exceeded only in $(1-\alpha)100\%$ of cases.
- **CVaR** can be though as a **weighted average** between α-**VaR** and the **losses exceeding it**.



Aerodynamic Design Optimisation *'toy'* problem

- Baseline Airfoil: NACA 2412
- Working conditions:
  - $M_\infty = 0.0$
  - $Re = 5 \times 10^5$
  - $C_l = 0.5$
- Flow solver: XFOIL
- 20 design variables, $\mathbf{w}$

$$
\begin{cases}
\min\limits_{\mathbf{w}} & C_d(\mathbf{w}) \\
\text{subject to:} & \\
& C_l = 0.5 \\
& t/c = 0.12 \\
& XTR_{LOW} \leq 0.95c \\
& TEA \geq 13^\circ \\
& LER \geq 0.007c
\end{cases}
$$



	$C_d \times 10^4$	α
NACA 2412	0.007266	2.411
Deterministic Opt.	0.005997	1.742

17.5% drag reduction

Aerodynamic Design Optimisation *'toy'* problem

What happen if **uncertainty** in the **shape** of the airfoil is **introduced**?

- Additional 20 uncertain variables, $\mathbf{z}$.
- 100 Monte Carlo Samples.

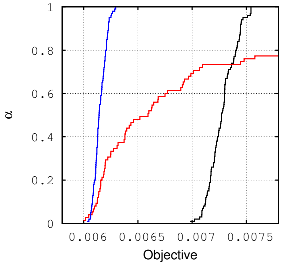
$$\begin{cases} \min\limits_{\mathbf{w}} & C_d(\mathbf{w},\mathbf{z}) \\ \text{subject to:} & \\ & C_l = 0.5 \\ & t/c = 0.12 \\ & XTR_{LOW} \leq 0.95c \\ & TEA \geq 13^\circ \\ & LER \geq 0.007c \end{cases}$$

Aerodynamic Design Optimisation *'toy'* problem

- NACA 2412: Probability 0.7 of having an increase of C_d w.r.t nominal value.
- Deterministic Optimum: A small change in shape is detrimental for the airfoil performance (huge increase of CVaR) $\rightarrow$ **Reliability Based Optimisation!**

$$\min_{\mathbf{w} \in W \subseteq \mathbb{R}^n} \mathrm{CVaR}^{0.9} \left(C_d(\mathbf{w}, \mathbf{z}) + P(\mathbf{w}, \mathbf{z}) \right)$$

- Robust Optimum:
  - Improve upper tail w/o deteriorating the lower.
  - 99 times more computationally expensive! $\rightarrow$ **Reduce CPU time!**



	$C_d \times 10^4$	α	$\mathrm{CVaR}^{0.9}$(Obj)
NACA 2412	0.007266	2.411	0.007496
Deterministic Opt.	0.005997	1.742	227.187
Robust Opt.	0.006117	1.662	0.006250

Efficient use of risk measures

- Sophisticate risk functions may require a very dense sampling and, hence, may result to be computationally intensive
- Sometimes importance sampling may be strategic to reduce the number of samples at an acceptable level.
- Stochastic collocation and surrogate modeling may also be very useful.
- Here we explore the effect on the efficiency of the risk function calculation process by choosing in a targeted (and deterministic) way the sample on which the risk function is calculated.

Robust Aerodynamic Design of a Blended Wing Body (BWB) aircraft central section.

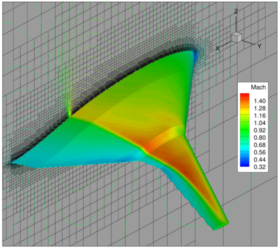
Design flow conditions

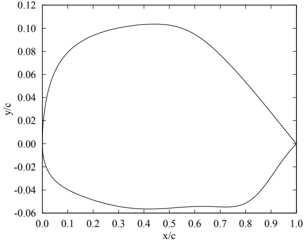
Parameters	*Values*
Mach	0.8
Reynolds	173.52×10^6
L_{ref}	33.5 m
AoA	-2.86°
C_L	0.10

Airfoil geometric characteristics

Parameters	*Values*
t/c	0.16
Leading Edge Radius (LER)	0.0156
Trailing Edge Angle (TEA)	27.57°
t/c at 85% chord (TAT)	0.083

Note: baseline configuration is a deterministically optimized airfoil with a constraint on the pitching stability behaviour.





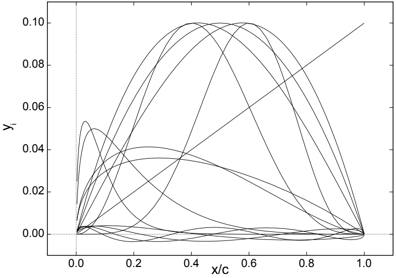
Airfoil Shape Parameterization

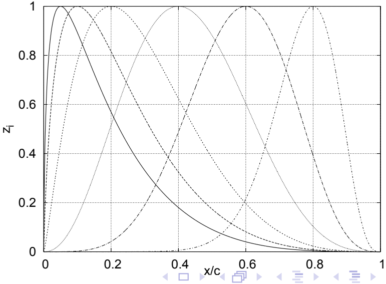
$$y(s) = k\left(y_0(s) + \sum_{i=1}^{n} w_i y_i(s)\right) + \sum_{j=1}^{m} U_j z_j(s),$$

$$x(s) = x_0(s),$$

$$z_j(s) = \sin^3\left(\pi x^{\frac{\log 0.5}{\log s_{b_j}}}\right)$$

- Initial shape, $(x_0(s), y_0(s))$
- Scale factor, $k \rightarrow$ max. thickness
- Modification functions, $y_i(s)$
- Design parameters, $w_i \in [-6, 6]$
- Hicks-Henne bump functions, $z_j(s)$





Geometrical and Operational Uncertainties

- The uncertainty of the wing shape is represented by a uniform random perturbation U_j that is added to the current shape functions.
- The uncertainties in the operational parameters Mach and AoA are modelled as four parameter beta distribution.

$$f(y;\alpha,\beta) = \frac{\gamma(\alpha+\beta)(y)^{\alpha-1}(1-y)^{\beta-1}}{\gamma(\alpha)\gamma(\beta)}$$

$$y = (x - \mathrm{loc})/\mathrm{scale}$$

Mach:
α=2, β=2,
scale=0.04, loc=0.78

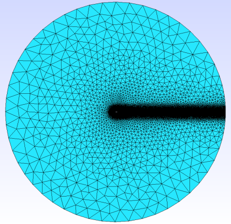
AoA:
α=2, β=2,
scale=0.30, loc=-0.15

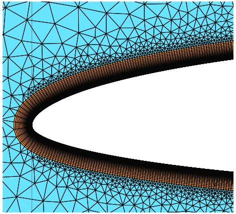
Uncertainty	Range	Distribution
Mach, M	$[0.78\ ,0.82]$	BETA
Angle of Attack, $\Delta\alpha$	$[-0.15^\circ, 0.15^\circ]$	BETA
Geometry, U_j	$[-0.0007\ ,0.0007]\ ,\ j=1,\dots,12$	UNIFORM

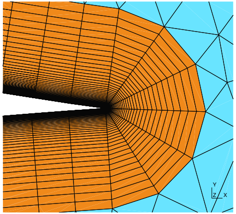
Numerical analysis tools

Automatic grid generation for RANS analysis ($\sim$ 160000 cells)

- Wake
- Boundary layer
- Shock waves
- *Corner points*







Finite volumes CFD RANS analysis

- "Spalart-Allmaras" model
- II order *Monotone Upstream-Centered Scheme for Conservation Law*
- Adaptive CFL number

Deterministic Design Optimization Problem

- Transonic airfoil section design. Drag reduction with geometric and aerodynamic constraints:

$$
\begin{cases}
\begin{aligned}
\min_{\mathbf{w}} \quad & C_d(\mathbf{w}) \\
\text{subject to:} \quad & \\
& t_{\%} = 16.00 \\
& \mathrm{LER} \geq 0.00781 \\
& \mathrm{TEA} \geq 22^\circ \\
& \mathrm{TAT} \geq 0.06658 \\
& C_l = 0.1; \\
& C_m \geq 0.01 \\
& C_m \leq 0.02 \\
& \mathrm{error} = 0
\end{aligned}
\end{cases}
$$

Deterministic Design Optimisation Problem

The penalty approach is used to account for constraints:

$$\min_{\mathbf{w}\in W\subseteq\mathbb{R}^n} C_d(\mathbf{w}) + P(\mathbf{w})$$

with

$$\begin{aligned} P(\mathbf{x}) \quad = \quad & k^1 p^+(\mathrm{LER}, 0.00781) + \\ & k^2 p^+(\mathrm{TEA}, 22.0^\circ) + k^3 p^+(\mathrm{TAT}, 0.06658) + \\ & k^4 p^+(C_m, 0.01) + k^4 p^-(C_m, 0.02) + k^5 p^+(\mathrm{error}, 0) \end{aligned}$$

All the constraints except those regarding the lift coefficient and the maximum airfoil thickness to chord ratio are quadratic penalties:

$$p^+(x,y) = \begin{cases} 0 & \text{if } \; x \geq y \\ (x-y)^2 & \text{if } \; x < y \end{cases} \qquad \text{and} \qquad p^-(x,y) = \begin{cases} (x-y)^2 & \text{if } \; x \geq y \\ 0 & \text{if } \; x < y \end{cases}$$

Robust Optimization Problem Setup

The introduction of the random variables causes a functional dependence in the QoI, which is now a function of functions. The CVaR risk function, at confidence level set to 0.9, is used to map the QoI into $\mathbb{R}$.

$$\min_{\mathbf{w} \in W \subseteq \mathbb{R}^n} \mathrm{CVaR}^{0.9}\left(C_d(\mathbf{w}, \mathbf{z})\right) + P(\mathbf{w})$$

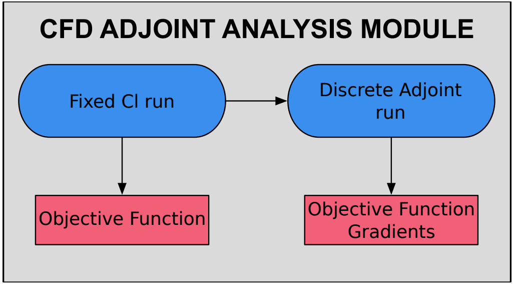
We are interested in evaluating the impact of random perturbations only on drag force, so constraints are computed at the nominal values of the design parameters, without taking into account the effects of uncertainties.

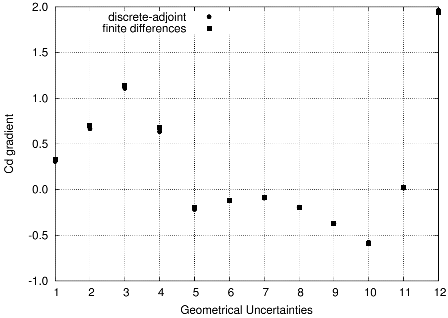
Gradient Based ECDF approximation — Intrusive if Adjoint is used

Strategy:

- RANS adjoint solution returns the gradients of the QoI w.r.t the uncertainty variables almost at the cost of one RANS flow solution.
- A linear approximation of the QoI is built by means of the extracted gradients.
- Empirical Cumulative Distribution Function (ECDF) is calculated.
- CVaR is estimated.

Computational Model Chain - QoI approximation





QoI linear approximation:

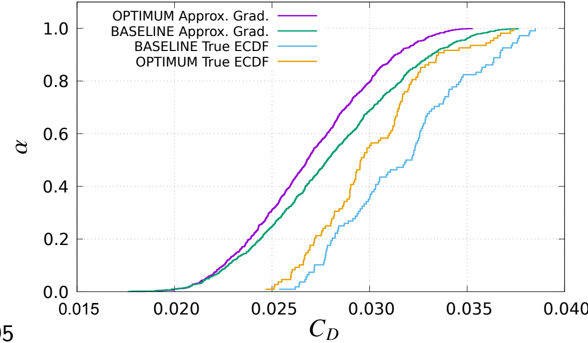
$$q(\mathbf{z}) \approx q(\mathbf{z}_0) + \sum_{i=1}^{n} \frac{\partial q(\mathbf{z}_0)}{\partial z^{(i)}} \left(z^{(i)} - z_0^{(i)} \right)$$

where $\mathbf{z}$ is the vector of the uncertain variables: $\mathbf{z} = [M, \Delta\alpha, U_j]$ (airfoil robust design).

CDF and CVaR comparison of baseline and optimal solution

- ECDF based on gradient approximation are estimated with 1000 samples during optimisation.
- True ECDF are obtained using 120 samples in the result analysis phase.

- A remarkable improvement of the upper tail is obtained, while a deterioration of the lower tail is avoided (advantage w.r.t classical approaches based on μ and σ).
- Despite a shift of the approximated solution, the trend of the true ECDF is captured, therefore the approximated $\mathrm{CVaR}^{0.9}$ is perfectly usable for robust optimisation.
- Confidence Intervals (CI) calculated with Bootstrap technique.



0.95

	Approx. Grad. ECDF			True ECDF		
	$\mathrm{CVaR}^{0.9}$	CI low	CI up	$\mathrm{CVaR}^{0.9}$	CI low	CI up
Baseline airfoil	0.0347	0.0343	0.0351	0.0375	0.0368	0.0380
Robust optimized airfoil	0.0327	0.0324	0.0330	0.0358	0.0344	0.0368

CVaR approximation through Gaussian Processes — non intrusive

- The regression method based on **Gaussian processes** was **used** to derive an **approximation** of the empirical cumulative distribution function (**ECDF**) for the QoI (the c_d in these benchmark cases).
- After that, the **statistics of interest**, such as mean and standard deviation, are **calculated from** the **approximation** of the **ECDF** obtained with the GPs.
- The approach based on **Gaussian processes** is here **implemented** in a very **simple way**, without resorting to sophisticated techniques such as sparse Gaussian processes or adaptive sampling.

Gaussian Processes

A Gaussian process defines a distribution of functions $p(f)$, with $f : X \mapsto \mathbb{R}$, such that by taking any finite number of random variable samples, $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \subset X$, the marginal distribution over that finite subset $p(\mathbf{f}) = p(\{f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n)\})$ is a multivariate Gaussian probability distribution.

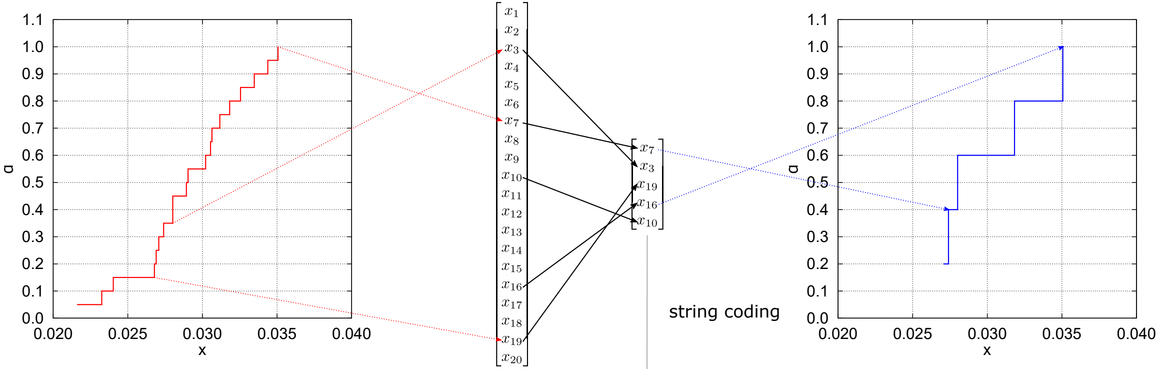
The process is completely defined by specifying a mean function $\mu(\mathbf{x})$ and a covariance function, or kernel, $K(\mathbf{x}_i, \mathbf{x}_j; \boldsymbol{\theta})$, where $\boldsymbol{\theta}$ is a vector of parameters that can be learned from data to obtain regression.

The covariance function here used has the following form:

$$\begin{aligned} K(\mathbf{x}_i, \mathbf{x}_j; \boldsymbol{\theta}) \quad = \quad \nu_1 \quad & \exp\left[-\frac{1}{2} \sum_{\ell=1}^{L} \frac{\left(x_i^{(\ell)} - x_j^{(\ell)} \right)^2}{r_\ell^2} \right] \\ & + \nu_2 + \delta_{ij} N(\mathbf{x}_i; \boldsymbol{\theta}) \end{aligned}$$

with $x^{(\ell)}$ the ℓ-th component of vector $\mathbf{x}$. The vector of hyperparameters is given by $\boldsymbol{\theta} = \{\nu_1, \nu_2, r_1, \ldots, r_L\}$ and N defines the noise model

Algorithm coding



$$[7, 3, 19, 16, 10]$$

Optimisation algorithms

- **GP training** → simple Genetic Algorithm (GA)

	Generations	Population	Crossover triggering probability [%]	Bit-mutation [%]
#1	16	120	100	2.4
#2	30	240	80	1.2
#3	150	240	80	1.2
#4	200	240	80	1.2

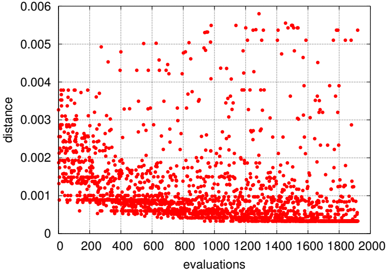
  The GA uses a Bit string encoding with Gray code.
  The Crossover operator is the classical one-point binary with given triggering probability.
  Bit-mutation: probability of changing the state of a single bit.

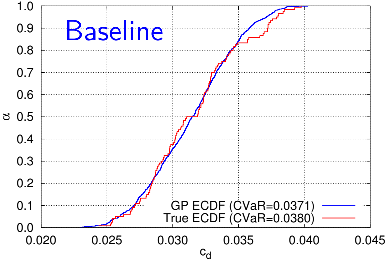
- **Robust optimisation run** → Covariance Matrix Adaptation Evolution Strategy (CMA-ES)

Maximum evaluations	Population size	Initial standard deviation
801	8	0.02

Preliminary GP Training

- PURPOSE: characterization of the deterministic solution robustness.
- Monte Carlo sampling of the uncertain variables → ECDF with 120 Hi-Fi samples.
- The GA encodes the selection of 5 elements extracted from the Hi-Fi ECDF.
- The GP constructs a response surface using these 5 elements and generates an approximated ECDF with a 1000 Monte Carlo samples.
- The objective function is the distance of this approximated ECDF from the original one.





- OUTPUT: 5 set of uncertain variables that minimise the distance.

Gaussian Process approximator adaptive refinement

- **CVaR** is **not** always **well approximated** $\rightarrow$ introduce the **minimisation** of the **difference** between **CVaRs** computed with **MC sample** and **CVaRs** computed with **GP** ($\overline{\mathrm{CVaR}}$) as a **new term** in the **objective function** for the training phase.
- **Small error** in CVaR **estimation** with GP $\rightarrow$ **lead** to the **overturning** of the **order relationship**: e.g Monte Carlo sampling indicates $\mathrm{CVaR}_1 < \mathrm{CVaR}_2$ and the GP approximation $\overline{\mathrm{CVaR}}_1 > \overline{\mathrm{CVaR}}_2$. IMPORTANT for OPTIMISATION!
- Introduce a penalty term $\rightarrow$ Consider the set of pairs (CVaR,$\overline{\mathrm{CVaR}}$) and reorder so that $\mathrm{CVaR}_i \leq \mathrm{CVaR}_{i-1}$

$$P_{\mathrm{tset}} = w \sum_{i=2}^{n} \mathbb{1}_C \left(\overline{\mathrm{CVaR}}_i > \overline{\mathrm{CVaR}}_{i-1} \right)$$

$$\mathbb{1}_C(x) := \begin{cases} 1 & \text{if } x \in C, \\ 0 & \text{if } x \notin C, \end{cases}$$

Example of iterative optimisation process

Step 1 — Preliminary GP training: baseline ECDF.

Step 2 — First robust optimisation run

Step 3 — Gaussian Process retraining: 4 ECDF training set.

Step 4 — Second robust optimisation run

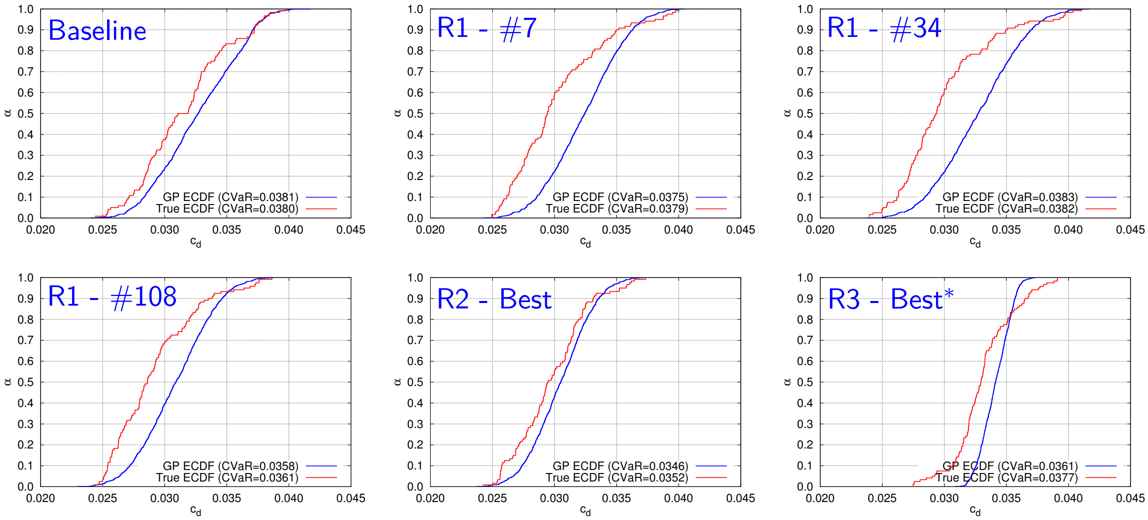
Step 5 — Third Gaussian Process retraining: 5 ECDF training set.

Step 6 — Third robust optimisation run

Step 7 — Fourth Gaussian Process retraining: 6 ECDF training set.

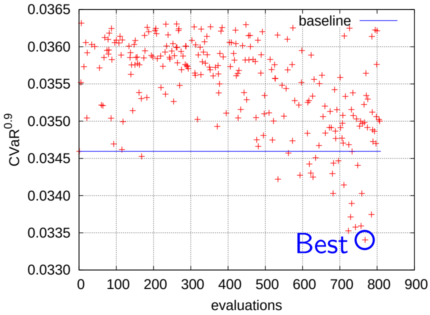
Step 8 — Fourth robust optimisation run

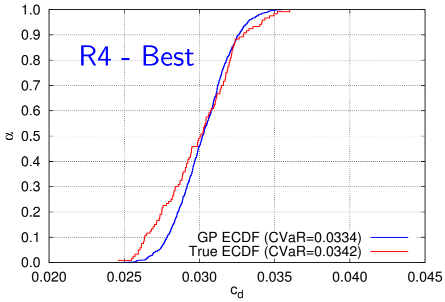
Final Gaussian Process retraining/refinement



Final Robust Optimisation Run

- Two phases: the first in which optimization is stagnant. The second in which the optimizer find an exploitable direction in the optimization process.
- ECDFs show an optimal agreement.

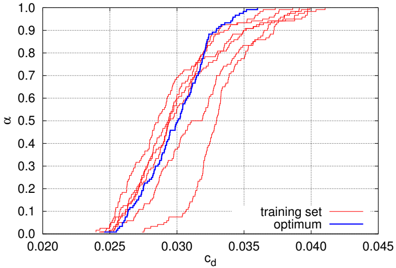


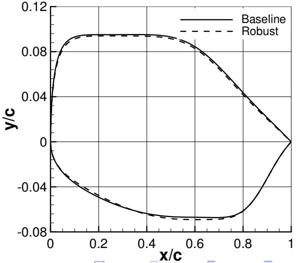


Final Robust Optimisation Run

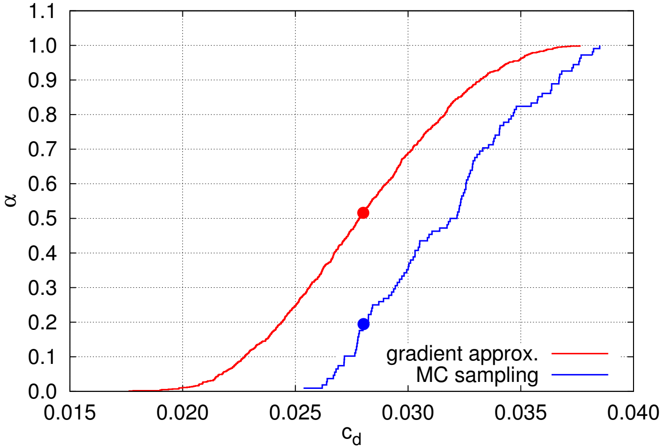
- The improvement calculated on the Hi-Fi distribution is 10% and the predicted improvement with the approximation is 12%.

Solution ID	Distance	CVaR	$\overline{\mathrm{CVaR}}$	penalty term
R1 #34	0.0029011	0.03821	0.03832	—
Baseline	0.0012991	0.03805	0.03810	0
R1 #7	0.0024264	0.03785	0.03748	0
R3 - Best*	0.0014308	0.03774	0.03608	0
R1 #108	0.0019234	0.03612	0.03579	0
R3 - Best	0.0008803	0.03550	0.03575	0
R2 - Best	0.0008981	0.03519	0.03460	0
R4 - Best	0.0005761	**0.03420**	**0.03341**	0



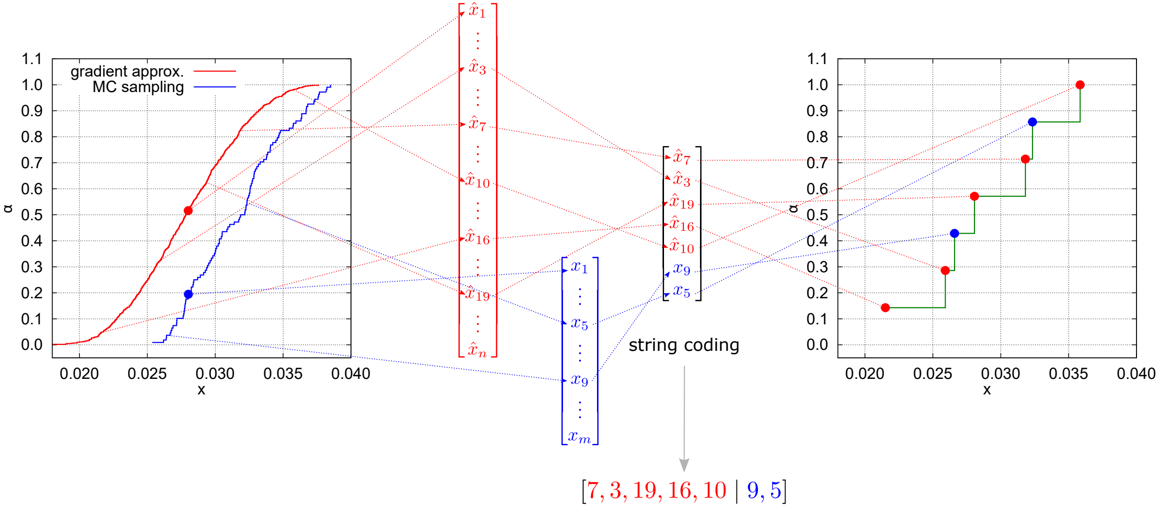


Hybrid Algorithm → intrusive + non-intrusive



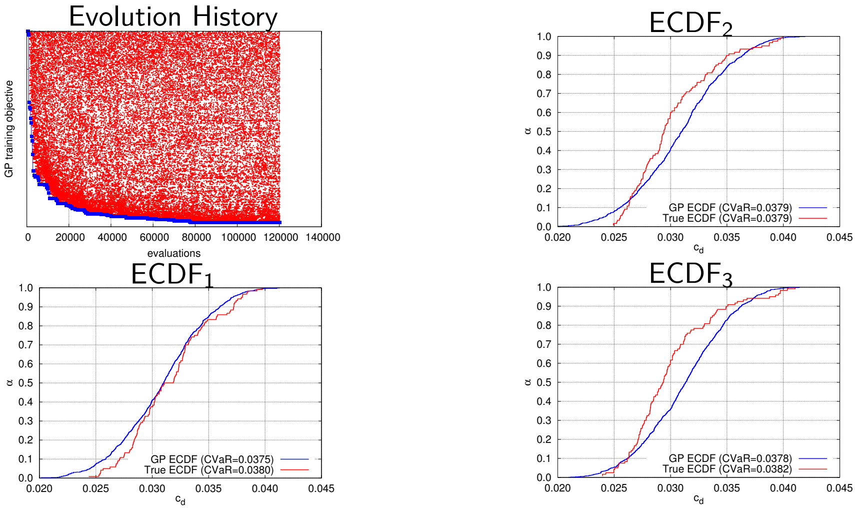
ECDF differences between MC sampling and gradient-based approximation.

Hybrid Algorithm → intrusive + non-intrusive



Algorithm scheme of the mixed gradient+GP approximator core

Hybrid Algorithm $\rightarrow$ intrusive + non-intrusive



Reduced Number of Samples from MC ECDF

Conclusions

- A robust optimisation approach based on CVaR can be successfully employed for aerodynamic design problems of industrial interest.
- The CVaR introduces the possibility of working asymmetrically on the ECDF: improving the upper tail without a deterioration of the lower.
- Both intrusive and non-intrusive approaches demonstrated their effectiveness for computational load reduction.
- The presented hybrid algorithm shows good potential for further reducing the computational load without deteriorating the quality of the approximation.

Thank you for your attention!
Any question?