ONERA
THE FRENCH AEROSPACE LAB

GdR Mascot-Num working meeting
May 11th, 2012 – Paris

Surrogate-based robust optimization for a combustion problem

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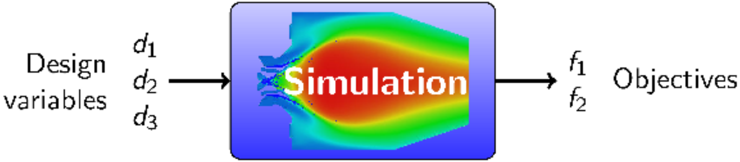
Optimize a system's performance

Reduce pollutant emissions of a turbomachine combustion chamber



$$\underset{\mathbf{d}}{\text{minimize}} \ \{f_1(\mathbf{d}), f_2(\mathbf{d})\}$$

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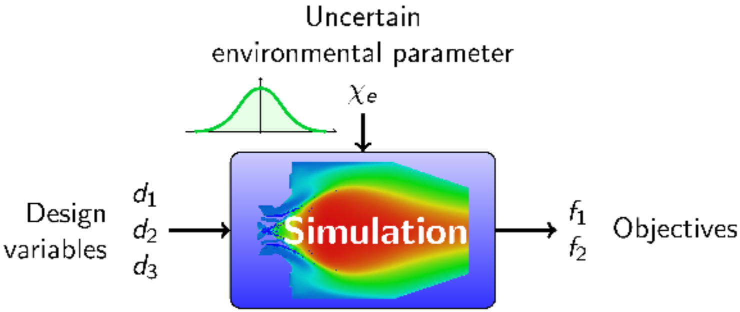
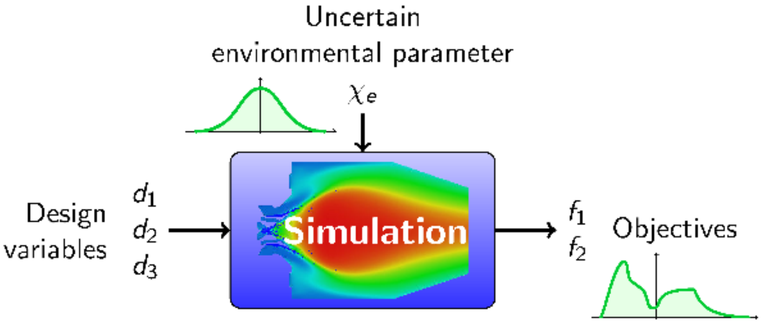


$$\underset{\mathbf{d}}{\text{minimize}} \; \{f_1(\mathbf{d}), f_2(\mathbf{d})\}$$

Introduction

Optimize a system's performance

Reduce pollutant emissions of a turbomachine combustion chamber



Stochastic problem: $\underset{\mathbf{d}}{\text{minimize}} \; \{f_1(\mathbf{d}, \chi_e), f_2(\mathbf{d}, \chi_e)\}$

Introduction

Main features of the problems to be solved:

- Expensive numerical simulations
- Multiobjective optimization problems
- Presence of uncertainties (probability distributions on $\mathbf{e}$ or $\mathbf{d}$)

$\rightarrow$ **development** of a surrogate-based adaptive strategy
for multiobjective robust optimization (PareBRO method)

Outline

Outline

Robust optimization

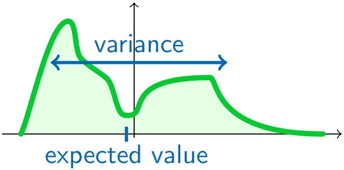
Find solutions insensitive to uncertainties

(Beyer and Sendhoff, 2007)

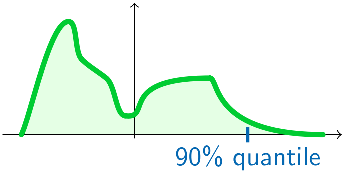
→ robustness quantification from the objectives probability distributions

Two main classes of robustness measurements ρ

Expectation-based measurements



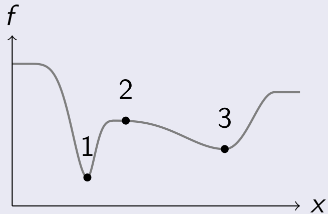
Quantile-based measurements



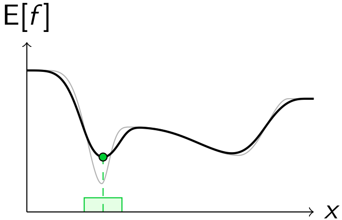
Robust problem: $\underset{\mathbf{d}}{\text{minimize}} \{\rho_1(f_1(\mathbf{d}, \chi_e)), \rho_2(f_2(\mathbf{d}, \chi_e))\}$

Expected value measurement

$$\mathrm{E}[f(\mathbf{d}, \chi_e)] = \int_{-\infty}^{\infty} f(\mathbf{d}, z) p_{\chi_e}(z) dz$$



initial objective

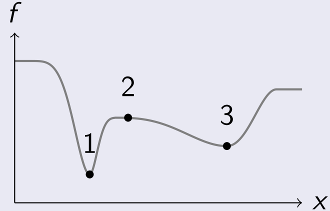


expected value

→ good average performance

Variance measurement

$$\mathrm{Var}(f(\mathbf{d},\chi_e)) = \mathrm{E}[f^2(\mathbf{d},\chi_e)] - \mathrm{E}^2[f(\mathbf{d},\chi_e)]$$



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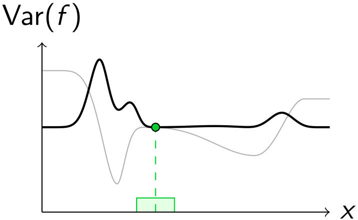


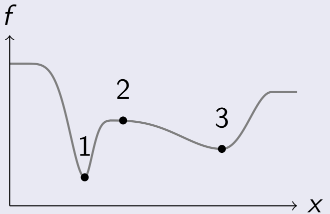
variance

$\rightarrow$ low performance variations

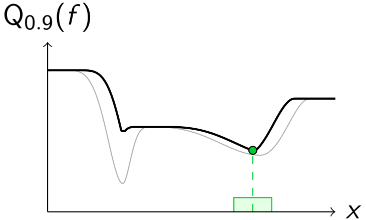
Robust optimization

k-quantile measurement

$$Q_k(f(\mathbf{d}, \chi_e)) = \inf\{q \in \mathbb{R} : P(f(\mathbf{d}, \chi_e) \leq q) \geq k\}$$



initial objective



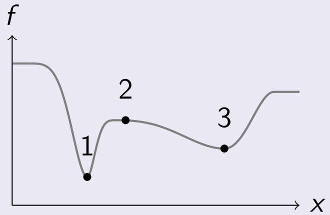
90% quantile

$\rightarrow$ performance guarantee

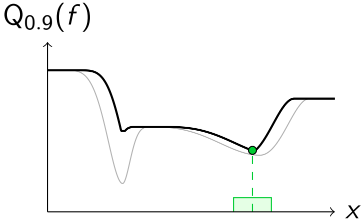
Robust optimization

k-quantile measurement

$$Q_k(f(\mathbf{d}, \chi_e)) = \inf\{q \in \mathbb{R} : P(f(\mathbf{d}, \chi_e) \leq q) \geq k\}$$



initial objective



90% quantile

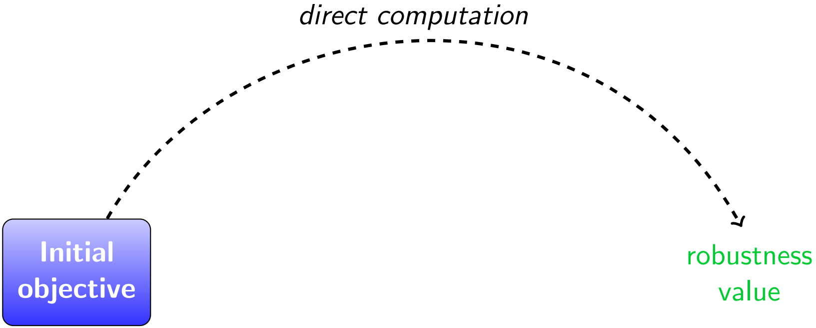
$\rightarrow$ performance guarantee

Choose a measurement based on the qualities expected

Robust optimization

Robustness measurement computation

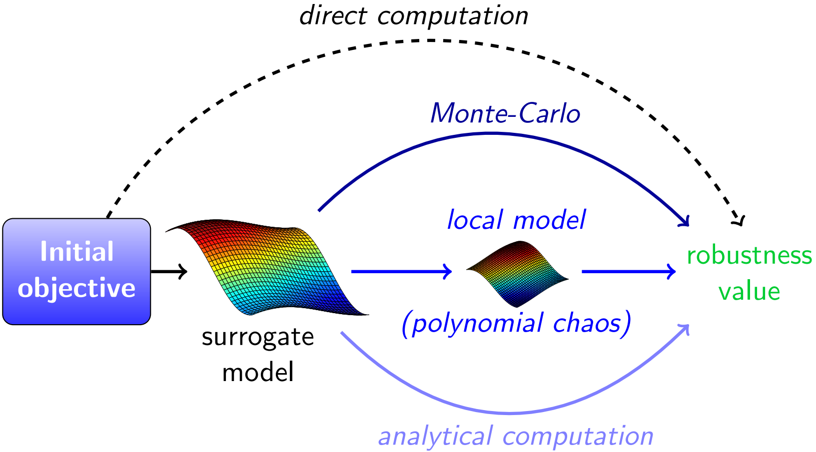
$\rightarrow$ need of surrogate models



Robust optimization

Robustness measurement computation

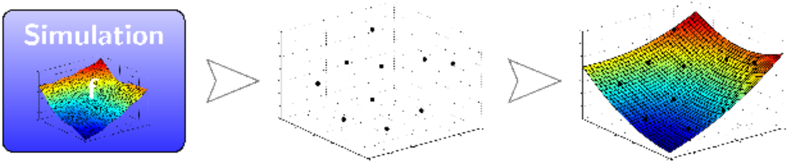
→ need of surrogate models



Robust optimization

Surrogate models

Polynomial approximations, neural networks, kriging, ...



Evaluation of samples $f(\mathbf{s})$ *(design of experiments)*

Surrogate model $\hat{f}$

Model hyperparameters θ optimized from the learning samples:

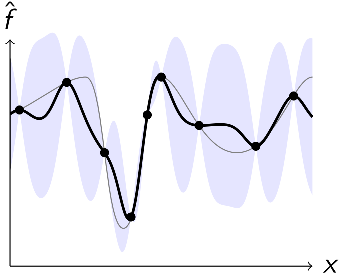
$$\underset{\theta}{\text{minimize}} \; ||f(\mathbf{s}) - \hat{f}_\theta(\mathbf{s})||$$

Fast evaluation, but approximation error (unknown)

Robust optimization

Kriging model (Krige, 1953)

Estimates confidence intervals on its own predictions (here at 95%)



Ordinary kriging model with a gaussian correlation function:

$$\hat{f}(\mathbf{x}) = a_0 + \sum_i a_i \prod_j e^{-\theta_j (x_j - s_j^i)^2}$$

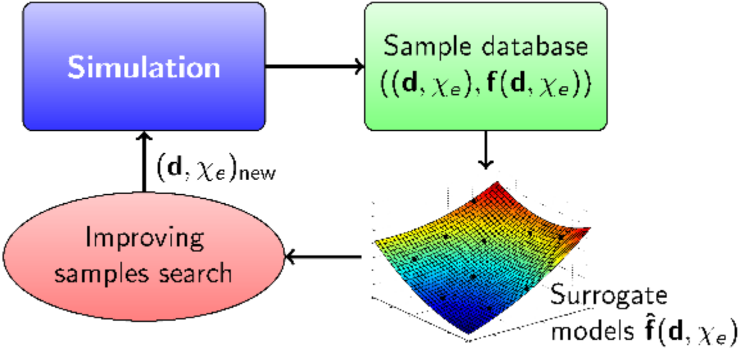
Exact analytical expression for the expected value and variance measurements with their confidence interval (Apley et al., 2006)

$$\mathrm{E}[\hat{f}(\mathbf{x})] = a_0 + \sum_i a_i \prod_j \int_{-\infty}^{\infty} e^{-\theta_j (x_j - s_j^i)^2} p_{\chi_j}(x_j) dx_j$$

Control model error with few learning samples

Adaptive design of experiments strategies

→ looking for the most informative samples to be added



Example: EGO "Efficient Global Optimization" (Jones et al., 1998)

Robust optimization

Develop an enrichment method:

a) allowing to improve several models simultaneously (multiobjective context)

b) dedicated to robust optimization
$\rightarrow$ add samples $(\mathbf{d}, \chi_e)$ improving the prediction of optimal areas (in $\mathbf{d}$ space)

c) allowing to numerically simulate n samples in parallel

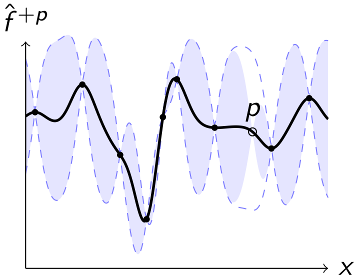
$\rightarrow$ **PareBRO method**

"Pareto Band Robust Optimization"

Outline

Sample “virtual” addition

Forecast the impact of a new learning sample **p** without having numerically simulated it



Kriging confidence intervals are estimated from:

$$\mathrm{Var}(\mathbf{x}) = \sigma_K^2 - \mathbf{c}(\mathbf{x})^T \mathbf{C}^{-1} \mathbf{c}(\mathbf{x})$$

→ add the sample **p** in the kriging model covariance matrix $\mathbf{C} = [\mathrm{Cov}(\mathbf{s}^i, \mathbf{s}^j)]_{i,j}$:

$$\mathbf{C}_2 = \begin{bmatrix} \mathbf{C} & \mathbf{c}(\mathbf{p}) \\ \mathbf{c}^T(\mathbf{p}) & \sigma_K^2 \end{bmatrix}$$

PareBRO method

a) Simultaneous improvement of several surrogate models

For each model $\hat{f}_i$, we aim at improving the solution $\mathbf{d}_i$ having the widest confidence interval CI_ρ

- Find the most poorly predicted solutions $\mathbf{d}_i$
- **Relative improvement** of the $\mathbf{d}_i$ confidence interval length when virtually adding the sample $\mathbf{p} = (\mathbf{d}, \chi_e)$ to model $\hat{f}_i$:

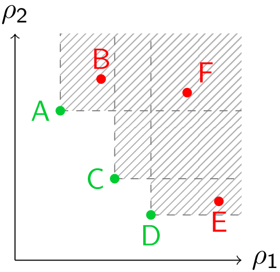
$$\mathrm{RI}_{\hat{f}_i}(\mathbf{p}) = \frac{|\,\mathrm{CI}_\rho(\hat{f}_i(\mathbf{d}_i))| - |\,\mathrm{CI}_\rho(\hat{f}_i^{+\mathbf{p}}(\mathbf{d}_i))|}{|\,\mathrm{CI}_\rho(\hat{f}_i(\mathbf{d}_i))|}$$

- Find the sample $\mathbf{p} = (\mathbf{d}, \chi_e)$ improving the confidence intervals of all $\mathbf{d}_i$:

$$\underset{\mathbf{p}}{\mathrm{argmax}} \sum_i \mathrm{RI}_{\hat{f}_i}(\mathbf{p})$$

b) Optimal areas improvement

Multiobjective optimization: compromises between the objectives



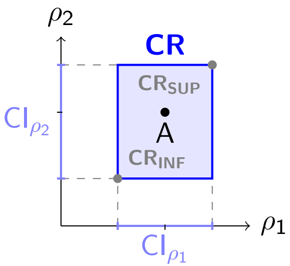
Pareto front: set of optimal solutions

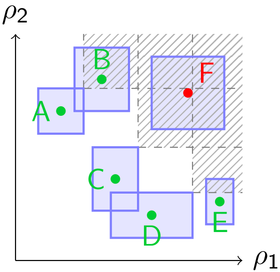
$$\text{“}\mathbf{X}\text{ dominates }\mathbf{Y}\text{”} \Leftrightarrow \mathbf{X} \prec \mathbf{Y} \Leftrightarrow \begin{cases} \forall i, \rho_i(\mathbf{X}) \leq \rho_i(\mathbf{Y}) \\ \exists j / \rho_j(\mathbf{X}) < \rho_j(\mathbf{Y}) \end{cases}$$

Not taking into account the models' confidence intervals
$\rightarrow$ some optimal solutions might be lost

ParèBRO method

The models 95% confidence intervals define a confidence region **CR** around the objective values





Pareto dominance taking confidence regions into account:

$$\mathbf{X} \prec_{CR} \mathbf{Y} \Leftrightarrow \mathbf{CR_{SUP}}(\mathbf{X}) \prec \mathbf{CR_{INF}}(\mathbf{Y})$$

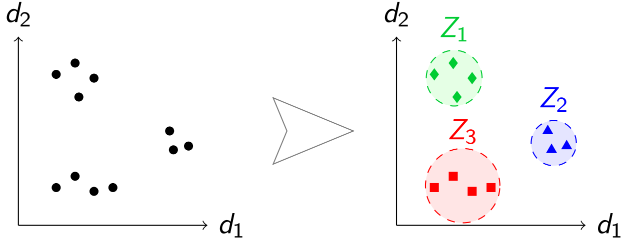
Pareto band: set of possibly optimal solutions
→ modified dominance integrated into NSGA-II

PareBRO method

c) Provide *n* improving samples to be simulated in parallel

Clustering of the Pareto band solutions (with *k-means*) in the design variable **d** space

→ identification of n possibly optimal areas Z_i

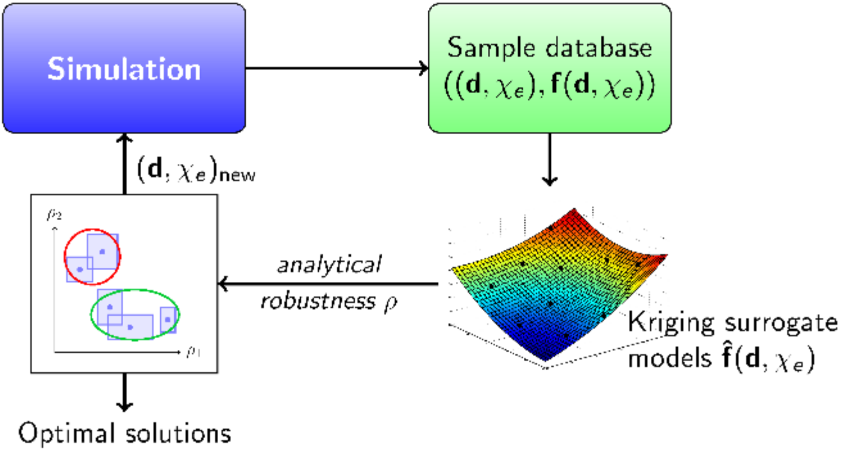


Search for an improving sample $\mathbf{p}_i$ in each area Z_i

(maximize the relative improvement RI of the points in Z_i having the widest confidence intervals)

PareBRO method

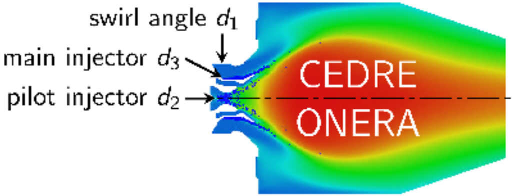
"Pareto Band Robust Optimization"



Outline

Robust optimization of an injection system

Combustion chamber with a multipoint injector



2D axisymmetric
2 days of computation
10 simulations in parallel

$$\underset{\mathbf{d}}{\text{minimize}} \; \{f_1(\mathbf{d}), f_2(\mathbf{d})\}$$

Reduce NO_x and CO **emissions**:

- minimize maximal temperature T_{max} f_1
- minimize output temperature standard deviation T_{stdev} f_2

Optimize three design variables:

- air intake swirl angle d_1
- pilot d_2 and main d_3 injectors positions

Robust optimization of an injection system

Injectors can clog partially

→ change in the fuel distribution between injectors, affecting the chamber performances

Uncertain environmental parameter $\chi_e \sim \mathcal{N}(0, \sigma^2_{\chi_e})$

$$\dot{m}_{\text{pilot}} = 0.15\ \dot{m}_{\text{total}} + \chi_e$$
$$\dot{m}_{\text{main}} = 0.85\ \dot{m}_{\text{total}} - \chi_e$$

Multiobjective robust optimization problem:

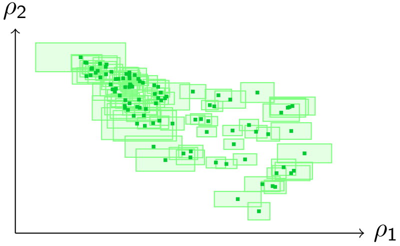
$$\underset{\mathbf{d}}{\text{minimize}}\ \{\rho_1(f_1(\mathbf{d}, \chi_e)), \rho_2(f_2(\mathbf{d}, \chi_e))\},$$
$$\text{with } \rho_i(f_i(\mathbf{d}, \chi_e)) = \mathrm{E}[f_i(\mathbf{d}, \chi_e)]$$

Analytical computation of the expected values on 2 kriging models $\hat{f}_1$ et $\hat{f}_2$ with 4 inputs (d_1, d_2, d_3 and χ_e)

Robust optimization of an injection system

Solving the combustion problem with PareBRO

Robustness values predicted in 100 points of search space:



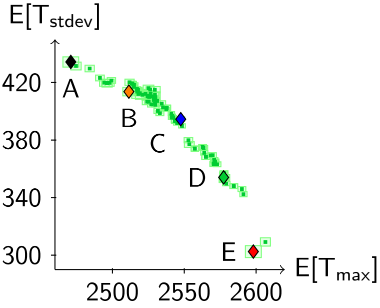
Before improvement (60 learning samples) | After improvement (200 learning samples)

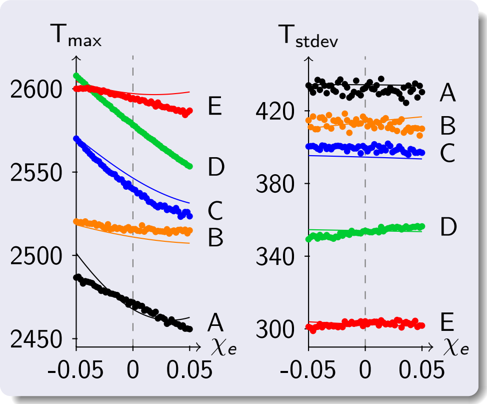
→ surrogate model precision has improved in the optimal areas

Robust optimization of an injection system

Final Pareto band obtained

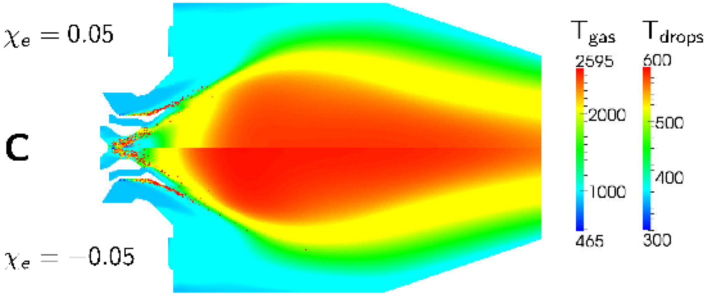
$\rightarrow$ analysis of 5 representative solutions
(with additional simulations for different values of χ_e)





Robust optimization of an injection system

Fuel distribution change effect



Gas temperature inside the combustion chamber

Outline

Conclusion

Better understanding of **uncertainty** management in optimization

PareBRO: surrogate-based robust optimization method

$\rightarrow$ deals with expensive simulations

$\rightarrow$ takes model error into account in a multiobjective context

$\rightarrow$ allows to simulate several samples in parallel

Robust solutions obtained from a limited number of simulations

Resolution of an **industrial** combustion problem

Conclusion

But **significant cost** for confidence intervals CI_ρ computation, even with surrogate models
(up to 6 hours to find 10 improving samples in our case)

Try to improve PareBRO **computing time**:

$\rightarrow$ Improve robustness measurement computation

$\rightarrow$ Experiment other surrogate models

$\rightarrow$ Consider other optimization algorithms

$\rightarrow$ Simplify the improving sample search

Expand to reliability-based optimization (**constraint** robustness)

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Thank you for your attention!

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