OPTIMAL UNCERTAINTY QUANTIFICATION OF A RISK MEASUREMENT FROM A COMPUTER CODE

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EDF R&D - Université Paul Sabatier

INTRODUCTION

INDUSTRIAL CONTEXT

We study a mock-up of a water pressured nuclear reactor during an intermediate break loss of coolant accident in the primary loop.

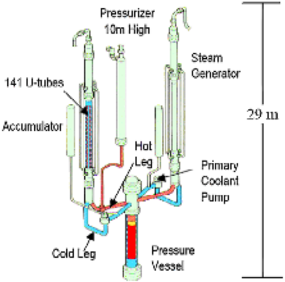


Figure – The replica of a water pressured reactor, with the hot and cold leg.

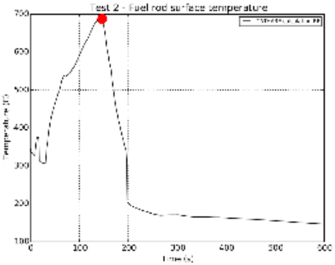
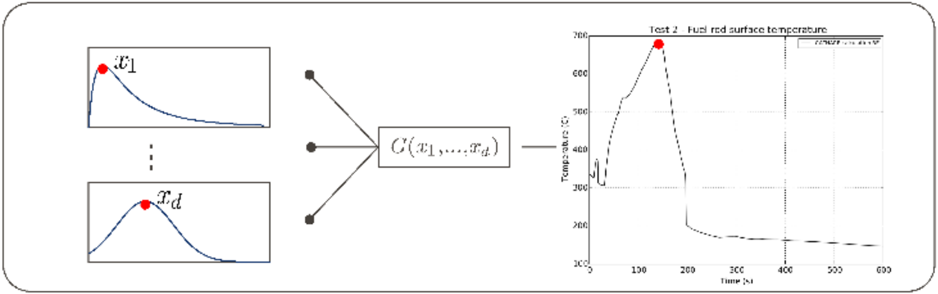


Figure – CATHARE temperature output for nominal parameters.

DETERMINISTIC METHOD

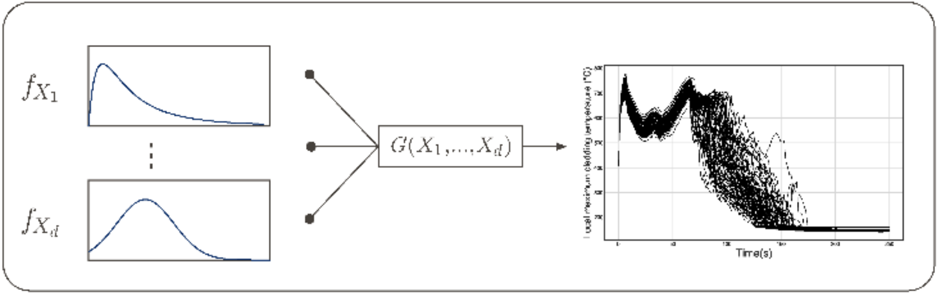
$$\underbrace{(x_1, \ldots, x_d)}_{\text{uncertain input parameters}} \rightsquigarrow \boxed{\texttt{COMPUTER MODEL}} \rightsquigarrow y$$



Our use-case is a thermal-hydraulic computer experiment (CATHARE), which simulates a intermediate break loss of coolant accident. The variable of interest is the peak cladding temperature.

PROBABILISTIC MODELIZATION

$$\underbrace{(X_1, \ldots, X_d)}_{\mu} \rightsquigarrow \boxed{\texttt{COMPUTER MODEL}} \rightsquigarrow Y$$



Let G be our computer code, the output distribution writes $F_{\mu}(h) = \mathbb{P}_{\mu}(G(X) \leq h)$.

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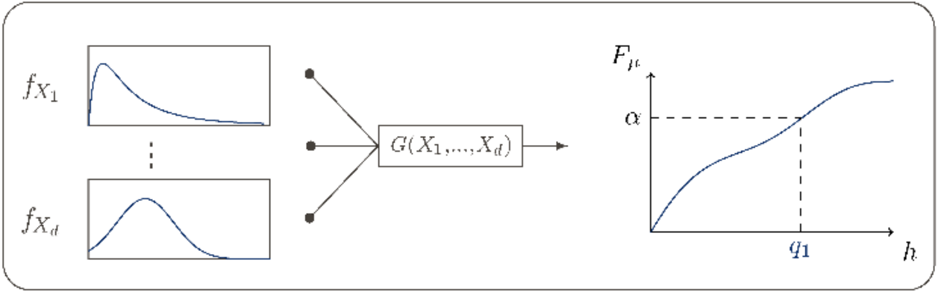

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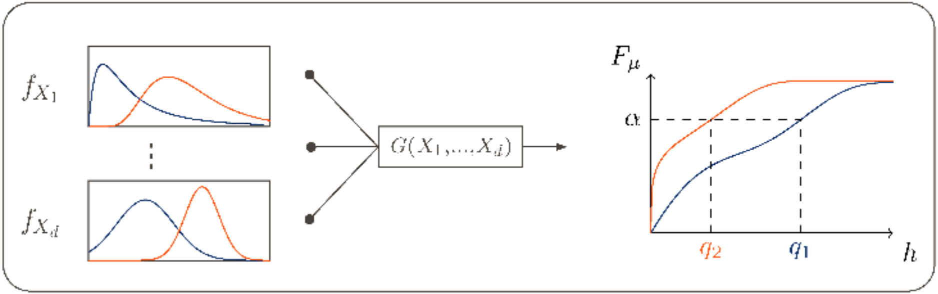

The quantity of interest (here a quantile) depends on the input distributions μ.

PROBABILISTIC MODELIZATION

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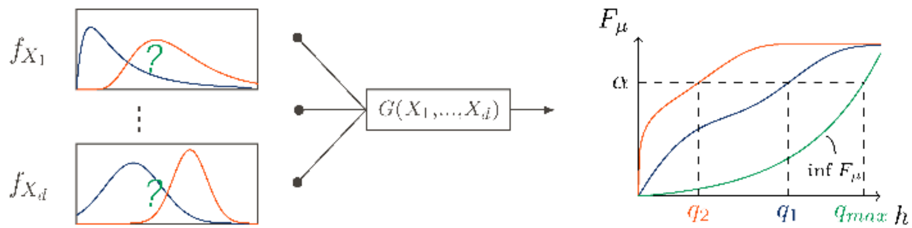


OUQ consists in finding the optimum of the quantity of interest over a set of input distribution $\mu \in \mathcal{A}$.

UNCERTAINTY MODELIZATION

We consider robustness by finding bounds on a quantity of interest ϕ

$$\mu \in \mathcal{P}(X) \mapsto \phi(\mu)$$

→ We optimize the quantity of interest over a measure space $\mathcal{A}$

$$\sup_{\mu \in \mathcal{A}} \phi(\mu)$$

→ The measure space $\mathcal{A}$ should be compatible with the data, it should effectively represent the uncertainty on the distribution.

THE MOMENT CLASS

In this work we will focus on two different optimization space.

→ The moment class :

$$\mathcal{A}^* = \left\{ (\mu_1, \ldots, \mu_d) \in \prod_{i=1}^{d} \mathcal{P}([l_i, u_i]) \mid \mathbb{E}_{\mu_i}[X^j] \leq c_i^{(j)} \ , \ j = 1, \ldots, N_i \right\} ,$$

→ and the unimodal moment class

$$\mathcal{A}^\dagger = \left\{ \text{Unimodal } \boldsymbol{\mu} \in \prod_{i=1}^{d} \mathcal{P}([l_i, u_i]) \mid \mathbb{E}_{\mu_i}[X^j] \leq c_i^{(j)} \ , \ j = 1, \ldots, N_i \right\} ,$$

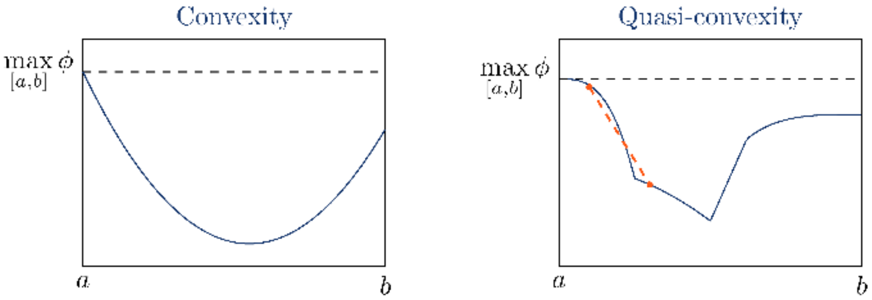
Problem : this is an optimization over an infinite non parametric space...

REDUCTION THEOREM

QUASI-CONVEX FUNCTION

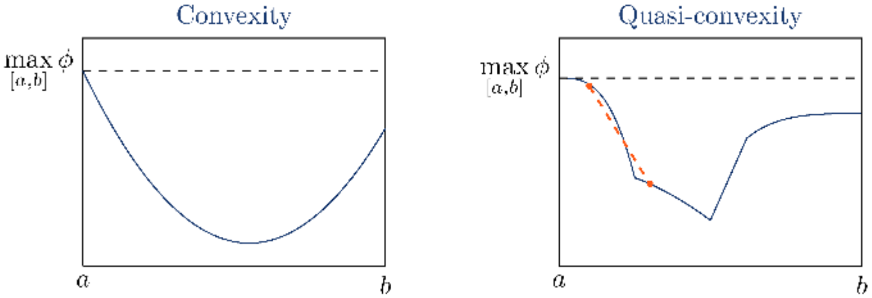
A function ϕ is said to be quasi-convex if

$$\phi(\lambda x + (1-\lambda)y) \leq \max\{\phi(x); \phi(y)\}$$



QUASI-CONVEX FUNCTION

From the Bauer maximum principle, a convex function on a compact convex set reaches its maximum on the extreme points



⇝The Bauer maximum principle remains true for quasi-convex function.

REDUCTION THEOREM

Reduction theorem

→ *The (unimodal) moment class is compact convex.*

→ *The quantity of interest ϕ is a quasi-convex lower semicontinuous function of the measure $\mu \in \mathcal{A}$*

Then,

$$\sup_{\mu \in \mathcal{A}} \phi(\mu) = \sup_{\mu \in \Delta} \phi(\mu) \ ,$$

where Δ is the set of extreme points of $\mathcal{A}$.

⇝ What are the extreme points of the (unimodal) moment class ?

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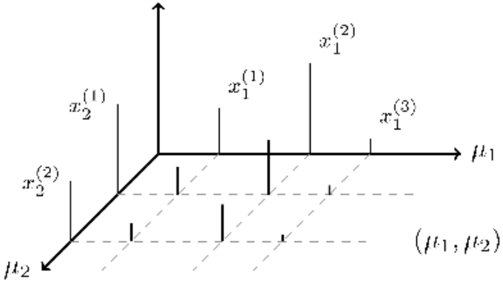
EXTREME POINTS CHARACTERIZATION (1/2)

Extreme points of the moment class

If you have N_i constraints on μ_i, then μ_i can be specified as a convex combination of at most $N_i + 1$ Dirac masses

$$\Delta^* = \left\{ \mu \in \mathcal{A}^* \mid \mu_i = \sum_{k=1}^{N_i+1} \omega_k \delta_{x_k},\ \ x_k \in [l_i, u_i] \right\}$$

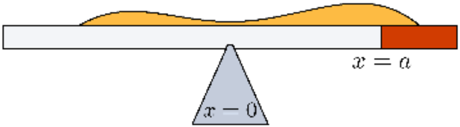


PHYSICAL ILLUSTRATION

First approach

You are given 1kg of sand to arrange however you wish on a seesaw balanced around $x = 0$.

→ How much mass can you pur on *the region* $\boldsymbol{x} \geq \boldsymbol{a}$?



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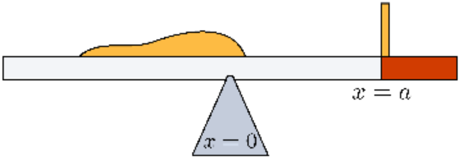

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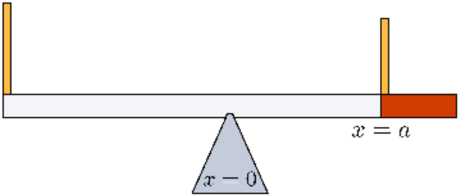


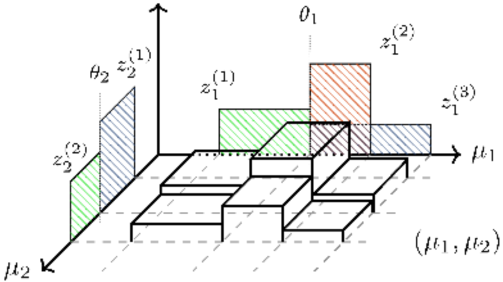
EXTREME POINTS CHARACTERIZATION (2/2)

Extreme points of the unimodal moment class

If you have N_i constraints on μ_i, then μ_i can be specified as a convex combination of at most $N_i + 1$ uniform distributions

$$\Delta^\dagger = \left\{ \mu \in \mathcal{A}^\dagger \mid \mu_i = \sum_{k=1}^{N_i+1} \omega_k \mathcal{U}(\theta_i, z_k), \;\; z_k \in [l_i, u_i] \right\}$$

where θ_i denotes the mode of μ_i.



REDUCTION THEOREM FOR A PROBABILITY OF FAILURE

Consider the quantity of interest to be a probability of failure (PoF).

$\rightsquigarrow$ it is a linear function of the input measure, thus is quasi-convex.

Over the moment class $\mathcal{A}^*$, the optimal PoF can be computed on the set of discrete finite input distributions :

$$\begin{aligned} \sup_{\mu \in \mathcal{A}^*} \phi(\mu) &= \sup_{\mu \in \mathcal{A}^*} F_{\mu}(h) \,, \\ &= \sup_{\mu \in \Delta^*} \mathbb{P}_{\mu}\big(G(X_1, \dots, X_d) \leq h\big) \,, \\ &= \sup_{\mu \in \Delta^*} \sum_{i_1=1}^{N_1+1} \cdots \sum_{i_d=1}^{N_d+1} \omega_{i_1}^{(1)} \dots \omega_{i_d}^{(d)} \, \mathbb{1}_{\{G(x_{i_1}^{(1)}, \dots, x_{i_p}^{(p)}) \leq h\}} \,. \end{aligned}$$

DISCRETE MEASURES

Let enforce N moment constraints on a measure $\mathbb{E}_\mu[X^j] = c_j$. OUQ theorem guaranties the optimal measure to be supported on at most $N+1$ points :

$$\mu = \sum_{i=1}^{N+1} \omega_i \delta_{x_i}$$

We have the following system of constraint equations :

$$\begin{cases} \omega_1 + \dots + \omega_{N+1} = 1 \\ \omega_1 x_1 + \dots + \omega_{N+1} x_{N+1} = c_1 \\ \vdots \qquad \qquad \vdots \qquad \vdots \\ \omega_1 {x_1}^N + \dots + \omega_{N+1} {x_{N+1}}^N = c_N \end{cases}$$

$\rightsquigarrow$ The weights are uniquely determined by the positions.

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⚠

GEOMETRICAL INTERPRETATION OF THE PARAMETRIZATION

Example : Let μ be supported on $[0,1]$ such that $\mathbb{E}_\mu[X] = 0.5$ and $\mathbb{E}_\mu[X^2] = 0.3$.

$$\Delta^* = \left\{ \mu = \sum_{i=1}^{3} \omega_i \delta_{x_i} \in \mathcal{P}([0,1]) \mid \mathbb{E}_\mu[X] = 0.5,\ \mathbb{E}_\mu[X^2] = 0.3 \right\} ,$$

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✓ $\mathbf{x} = (0.1, 0.4, 0.9)$ gives weights $\boldsymbol{\omega} = (0.05, 0.73, 0.22)$

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$$\mathcal{V}_{\Delta^*} = \left\{ \mathbf{x} = (x_1, x_2, x_3) \in [0,1]^3 \mid \mu = \sum_{i=1}^{3} \omega_i \delta_{x_i} \in \Delta^* \right\}$$

How to optimize over and explore the manifold $\mathcal{V}_\Delta$?

POSSIBLE WAYS OF OPTIMIZING

→ Optimization under constraints : the position and the weight must satisfy the Vandermonde system.

→ Optimization by rewriting the objective function : changing the parameterization of the problem so that the constraint are naturally enforced in the objective function.

⟶ Canonical moments allows to efficiently explore the set of optimization Δ^*.

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CANONICAL MOMENTS PARAMETERIZATION

CLASSICAL MOMENTS PROBLEM

$$\left(\frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \dots\right)$$

⇝ Moment sequence of $\mathcal{U}[0,1]$

$$\left(1, \frac{4}{3}, 2, \dots\right)$$

⇝ Moment sequence of $\mathcal{U}[0,2]$

Conclusion : there is no relation between the classical moments and the intrinsic structure of the distribution.

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Conclusion : there is no relation between the classical moments and the intrinsic structure of the distribution.

MOMENT SPACE

We define the moment space $M_n = \{\mathbf{c}_n(\mu) = (c_1, \ldots, c_n) \mid \mu \in \mathcal{P}([0,1])\}$

Given $\mathbf{c}_n \in \operatorname{int} M_n$, we define the extreme values

$$c^+_{n+1} = \max\{c : (c_1, \ldots, c_n, c) \in M_{n+1}\}$$
$$c_{n+1} = \min\{c : (c_1, \ldots, c_n, c) \in M_{n+1}\}$$

They represent the maximum and minimum value of the $(n+1)$th moment a measure can have, when its moments up to order n equal to c_n.

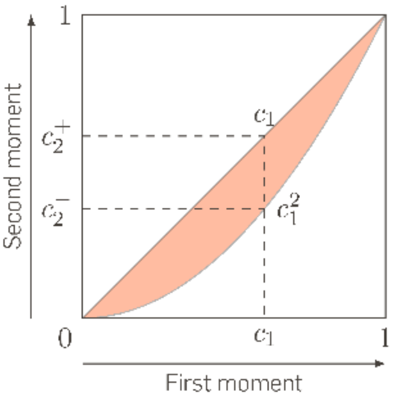

Figure : representation of M_2

CANONICAL MOMENTS

The nth canonical moment is defined as

$$p_n = p_n(\mathbf{c}) = \frac{c_n - c_n^-}{c_n^+ - c_n^-}$$

Properties of canonical moments

- $p_n \in [0, 1]$,
- The canonical moments are invariants by affine transformation. Which means we can always transform a measure supported on $[a, b]$ to $[0, 1]$

LINK BETWEEN SUPPORT AND CANONICAL MOMENTS

Given a measure $\mu = \sum_{i=1}^{n+1} \omega_i \delta_{x_i}$, we have two representations of the same polynomial P^*_{n+1} :

→ Its roots are the measure support points :

$$P^*_{n+1}(z) = \prod_{i=1}^{n+1} (z - x_i) \,.$$

→ Its coefficients are function of a sequence of the measure canonical moments $\mathbf{p} = (p_1, \ldots, p_{2n+1})$:

$$P^*_{n+1}(z) = \varphi_0(\mathbf{p}) + \varphi_1(\mathbf{p})z + \cdots + \varphi_{n+1}(\mathbf{p})z^{n+1} \,.$$

LINK BETWEEN SUPPORT AND CANONICAL MOMENTS

Given a measure $\mu = \sum_{i=1}^{n+1} \omega_i \delta_{x_i}$, we have two representations of the same polynomial P_{n+1}^* :

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EFFECTIVE PARAMETERIZATION

Let $\mu \in \Delta^* = \left\{ \sum_{i=1}^{n+1} \omega_i \delta_{x_i} \in \mathcal{P}([a,b]) \mid \mathbb{E}_\mu[X^j] = c_j,\ 1 \leq j \leq n \right\}$

EFFECTIVE PARAMETERIZATION

$$\mu \in \Delta^*$$

$\downarrow$ The support of μ is the roots of a polynomial $P^*_{n+1} = \prod_{i=1}^{n+1}(x - x_i)$

$$P^*_{n+1}$$

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$$P_{n+1}^* = \varphi_0(\mathbf{p}) + \varphi_1(\mathbf{p})z + \cdots + \varphi_{n+1}(\mathbf{p})z^{n+1}$$

$$\mathbf{p} = (p_1, \ldots, p_n, p_{n+1}, \ldots, p_{2n+1})$$

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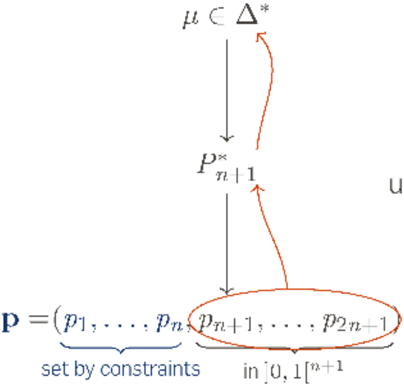
$$\mathbf{p} = (\underbrace{p_1, \ldots, p_n}_{\text{set by constraints}}, \underbrace{p_{n+1}, \ldots, p_{2n+1}}_{\text{in }]0,1[^{n+1}})$$

EFFECTIVE PARAMETERIZATION



We can explore the whole set Δ^* using a parameterization in $]0,1[^{n+1}$.

GENERATION OF ADMISSIBLE MEASURES

Theorem

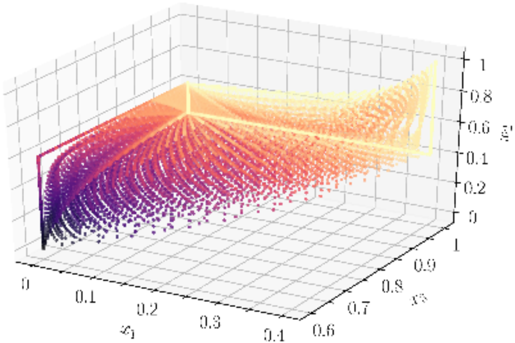
The manifold

$$\mathcal{V}_{\Delta^*} = \Big\{ \mathrm{x} = (x_1, \ldots, x_{n+1}) \in [0,1]^{n+1} \text{ s.t. } \mu = \sum_{i=1}^{n+1} \omega_i \delta_{x_i} \text{ satisfies the constraints} \Big\}$$

is an algebraic variety, it is the zero locus of the set of polynomials

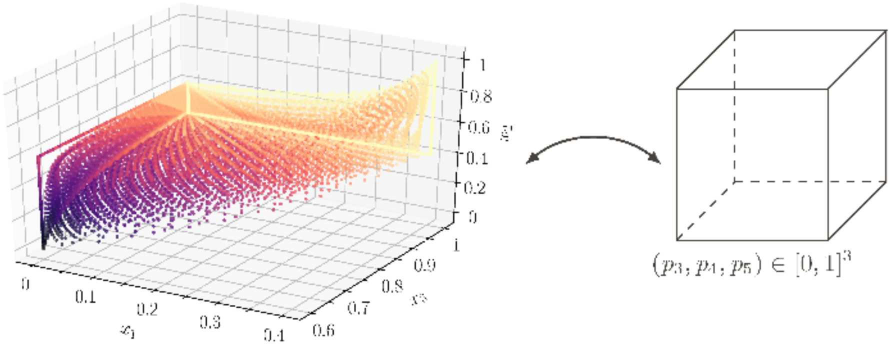
$$\Big\{ P^*_{n+1} \mid (p_{n+1}, \ldots, p_{2n+1}) \in [0,1]^{n+1} \Big\}$$

SET OF ADMISSIBLE MEASURES



- → Consider μ in $[0,1]$ and two moment constraints : $c_1 = 0.5$ and $c_2 = 0.3$ equivalent to $p_1 = 0.5$ and $p_2 = 0.2$.
- → We generate randomly $(p_3, p_4, p_5) \in [0,1]^3$ and compute for every sequence P_3^* whose roots constitute the coordinates of the points.
- → The point coordinates correspond to the support of a discrete measure in $\mathcal{A}$.

SET OF ADMISSIBLE MEASURES



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ALGORITHM

Algorithm 1 : P.O.F COMPUTATION

Inputs : - lower bounds, $\mathbf{l} = (l_1, \dots, l_d)$

- upper bounds, $\mathbf{u} = (u_1, \dots, u_d)$
- constraints sequences of moments, $\mathbf{c}_i = (c_i^{(1)}, \dots, c_i^{(N_i)})$ and its corresponding sequences of canonical moments, $\mathbf{p}_i = (p_i^{(1)}, \dots, p_i^{(N_i)})$ for $1 \leq i \leq d$.

function P.O.F($p_1^{(N_1+1)}, \dots, p_1^{(2N_1-1)}, \dots, p_d^{(N_d+1)}, \dots, p_d^{(2N_d+1)}$)

for $i = 1, \dots, d$ *do*

for $k = 1, \dots, N_i$ *do*

$$P_{i*}^{(k+1)} = (X - l_i - (u_i - l_i)(\zeta_i^{2k} + \zeta_i^{(2k+1)}))P_{i*}^{(k)} - (u_i - l_i)^2 \zeta_i^{(2k-1)} \zeta_i^{(2k)} P_{i*}^{(k-1)};$$

$x_i^{(1)}, \dots, x_i^{(N_i+1)} = \text{roots}(P_i^{*(N_i+1)});$

$\omega_i^{(1)}, \dots, \omega_1^{(N_i+1)} = \text{weight}(x_i^{(1)}, \dots, x_1^{(N_i+1)}, \mathbf{c}_i);$

return $\sum_{i_1=1}^{N_1+1} \dots \sum_{i_d=1}^{N_d+1} \omega_1^{(i_1)} \dots \omega_d^{(i_d)} \mathbb{1}_{\{G(x_1^{(i_1)}, \dots, x_d^{(i_d)}) \leq h\}};$

ILLUSTRATION

INDUSTRIAL CONTEXT

Our use-case is a thermal-hydraulic computer experiment (CATHARE), which simulates a intermediate break loss Of coolant accident. The variable of interest is the peak cladding temperature.

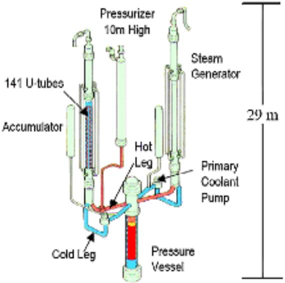


Figure – The replica of a water pressured reactor, with the hot and cold leg.

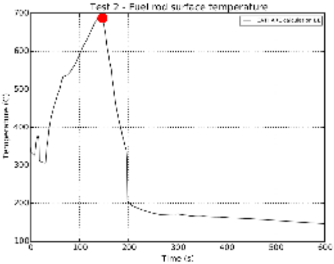


Figure – CATHARE temperature output for nominal parameters.

MOMENT CONSTRAINTS FOR CATHARE

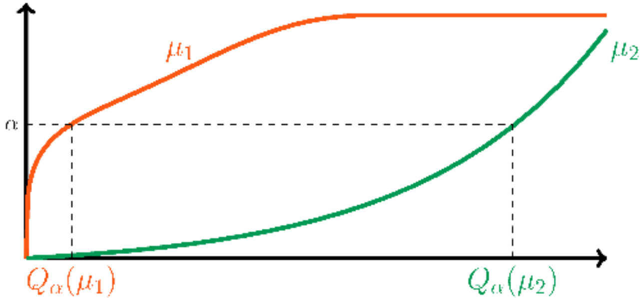
Variable	Bounds	Initial distribution (truncated)	Mean	Second order moment
$n°10$	$[0.1, 10]$	$LogNormal(0, 0.76)$	1.33	3.02
$n°22$	$[0, 12.8]$	$Normal(6.4, 4.27)$	6.4	45.39
$n°25$	$[11.1, 16.57]$	$Normal(13.79$	13.83	192.22
$n°2$	$[-44.9, 63.5]$	$Uniform(-44.9, 63.5)$	9.3	1065
$n°12$	$[0.1, 10]$	$LogNormal(0, 0.76)$	1.33	3.02
$n°9$	$[0.1, 10]$	$LogNormal(0, 0.76)$	1.33	3.02
$n°14$	$[0.235, 3.45]$	$LogNormal(-0.1, 0.45)$	0.99	1.19
$n°15$	$[0.1, 3]$	$LogNormal(-0.6, 0.57)$	0.64	0.55
$n°13$	$[0.1, 10]$	$LogNormal(0, 0.76)$	1.33	3.02

Table – Corresponding moment constraints of the 9 most influential inputs of the CATHARE model. Two moment constraints are enforced, that correspond to the mean and the variance of each input distribution.

QUASI-CONVEXITY OF THE QUANTILE (HEURISTIC)

Why is the quantile a quasi-convex function of the measure?

Let denote $Q_p(\mu)$ the quantile of order p of a distribution μ.



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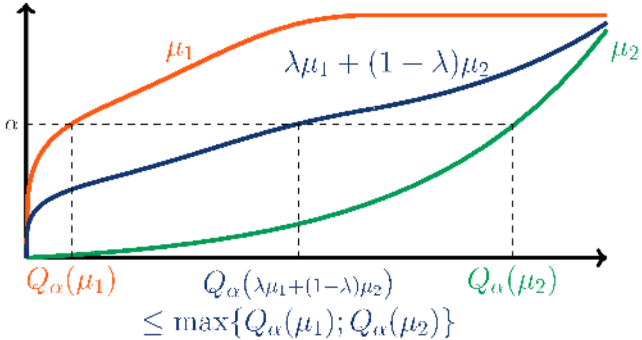

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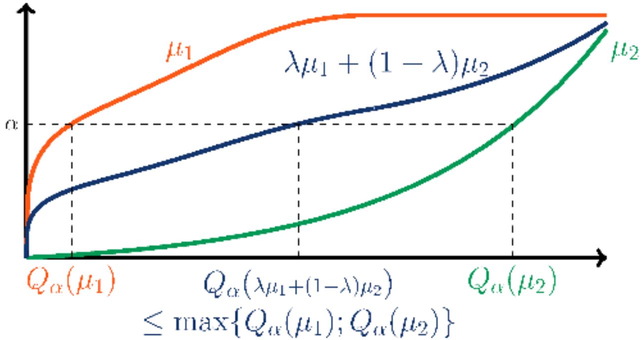
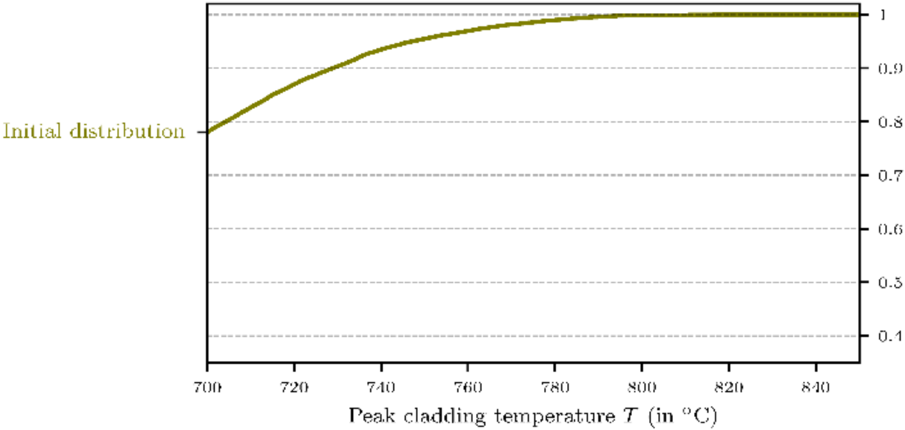


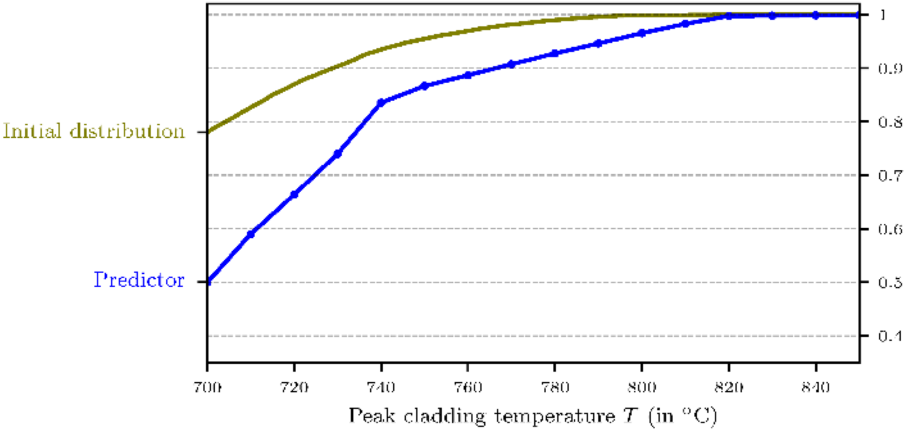
⇝ For the same reason, the superquantile is a quasi-convex function of the measure.

OPTIMIZATION FOR CATHARE



$$q_{init}^{0.95} = 760^{\circ}C$$

OPTIMIZATION FOR CATHARE



$$q_{init}^{0.95} = 760^{\circ}C \quad \rightsquigarrow \quad q_{optim}^{0.95} = 788^{\circ}C$$

UNCERTAINTY TAINTING THE METAMODEL (1/2)

We recall the probability of failure $F_\mu(h)$ is computed as

$$\begin{aligned}\inf_{\mu\in\mathcal{A}} F_\mu(h) &= \inf_{\mu\in\mathcal{A}} \mathbb{P}_\mu\big(G(X_1,\dots,X_d)\le h\big)\,,\\ &= \inf_{\mu\in\Delta} \sum_{i_1=1}^{N_1+1}\dots\sum_{i_d=1}^{N_d+1} \omega_{i_1}^{(1)}\dots\omega_{i_d}^{(d)}\,\mathbb{1}_{\{G(x_{i_1}^{(1)},\dots,x_{i_p}^{(p)})\le h\}}\,.\end{aligned}$$

$\rightsquigarrow$ The simple approach takes $G(\mathbf{x})$ as the predictor of the kriging metamodel $\mathscr{G}(\mathbf{x},\boldsymbol{\theta})$.

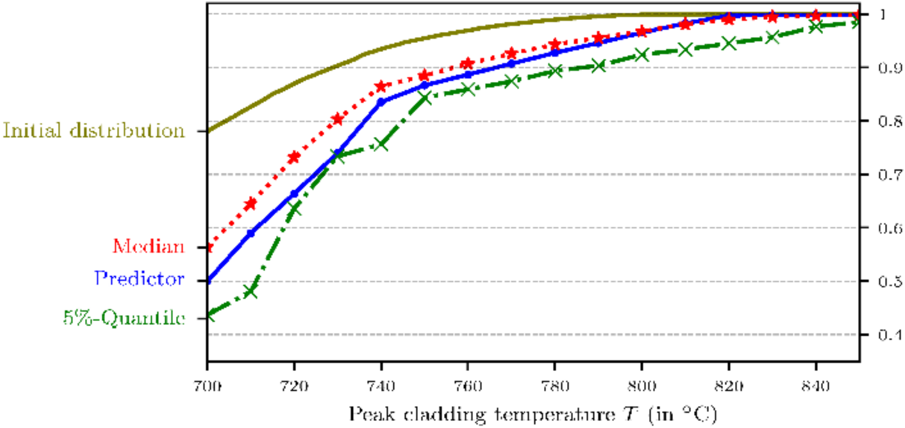
UNCERTAINTY TAINTING THE METAMODEL (2/2)

⇝ We propose to compute $F_\mu(h)$ for several trajectories of the metamodel, and minimize a quantile of the resulting sample.

$$\inf_{\mu \in \mathcal{A}} F_\mu(h, \boldsymbol{\theta}) = \inf_{\mu \in \mathcal{A}} \mathbb{P}_\mu\Big(\mathscr{G}(X_1, \dots, X_d, \boldsymbol{\theta}) \leq h\Big) \,,$$

$$= \inf_{\mu \in \Delta} \underbrace{\sum_{i_1=1}^{N_1+1} \cdots \sum_{i_d=1}^{N_d+1} \omega_{i_1}^{(1)} \dots \omega_{i_d}^{(d)} \, \mathbb{1}_{\{\mathscr{G}(x_{i_1}^{(1)}, \dots, x_{i_p}^{(p)}, \boldsymbol{\theta}) \leq h\}}}_{\text{get a sample for different realization of the gaussian process}} \,.$$

OPTIMIZATION FOR CATHARE



$$q_{init}^{0.95} = 760° C \quad \rightsquigarrow \quad q_{optim}^{0.95} = 788° C \quad \rightsquigarrow \quad q_{\substack{optim \\ robust}}^{0.95} = 830° C$$

CONCLUSION AND PERSPECTIVES

→ The reduction theorem gives the basis for numerical optimization of the quantity of interest.

→ The moment class and unimodal moment class have very interesting topological structure.

→ The canonical moment parameterization is well suited for exploring the extreme points, thus fastening the global optimization.

→ Inequality moment constraints can also be enforced.

CONCLUSION AND PERSPECTIVES

- → The reduction theorem gives the basis for numerical optimization of the quantity of interest.
- → The moment class and unimodal moment class have very interesting topological structure.
- → The canonical moment parameterization is well suited for exploring the extreme points, thus fastening the global optimization.
- → Inequality moment constraints can also be enforced.

- → The framework is limited to *classical* moment constraints. The quantile class is also interesting for engineering applications.
- → The raw global optimization could be refine for instance by computing gradient of the quantity of interest.
- → The computation is subject to the curse of dimensionality. Reducing the input dimension is a mandatory first step.

SOME REFERENCES

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THANK YOU FOR YOUR ATTENTION!