OPTIMAL UNCERTAINTY QUANTIFICATION OF A RISK MEASUREMENT ON MOMENT CLASS

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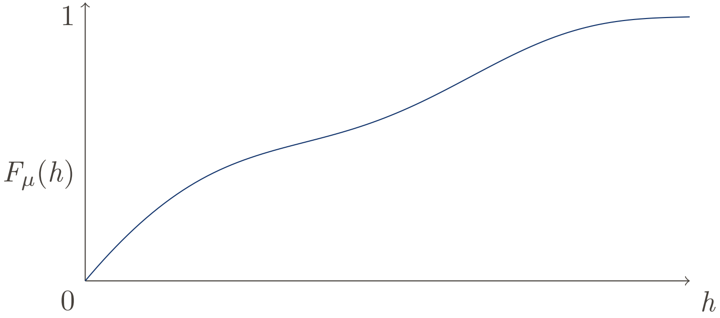
Sommaire

OUQ BASIS

NOTION OF ROBUSTNESS

Let G be our computer code, such that $F_\mu(h) = P_\mu(G(X) \leq h)$.



Inputs values are generated from an associated joint distribution, choosen thanks to an expert opinion.

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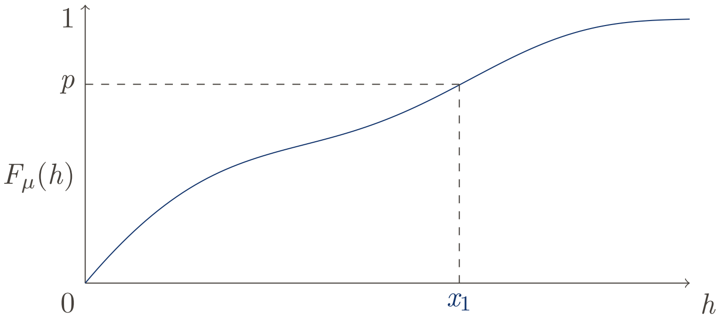

We are interested in a risk measurement, here a quantile of order p.

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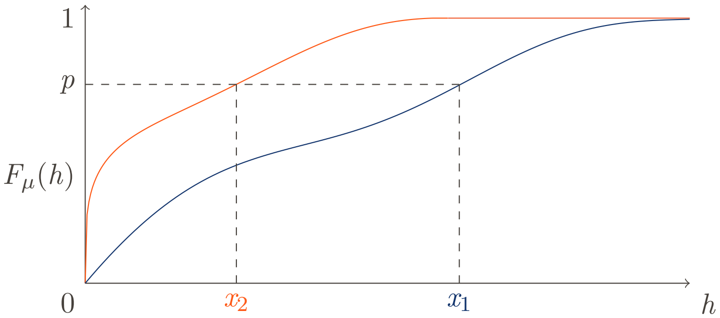

But if we change the associated joint distribution, the resulting quantile may differ.

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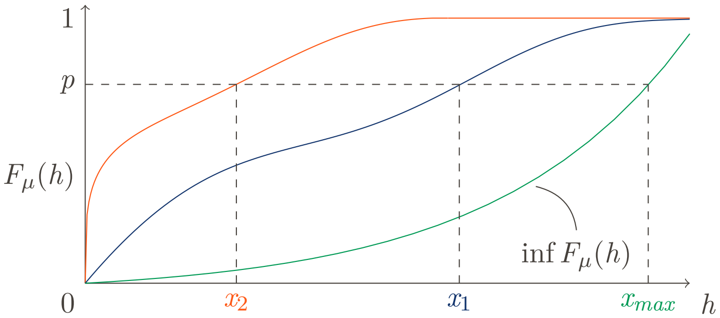

In order to be robust, we'd like to obtain the maximum quantile over a given class of measure.

DUALITY THEOREM

Let $\mathcal{A}$ be a class of measure. We are looking for the maximum quantile over this class.

DUALITY THEOREM

$$\underbrace{\sup_{\mu\in\mathcal{A}}\left[\inf\{h>0;\ F_\mu(h)\geq p\}\right]}_{\text{max quantile over all cdf}} = \underbrace{\inf\left\{h>0 \mid \inf_{\mu\in\mathcal{A}} F_\mu(h)\geq p\right\}}_{\text{quantile of the lowest cdf}}$$

RESULTING PROBLEM

We will therefore be looking for the lowest CDF

$$\inf_{\mu \in \mathcal{A}} F_\mu(h)$$

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

REDUCTION THEOREM

EXTEME POINTS OF MOMENT SETS

- → Let $\mathcal{X} = \{1, 2, 3\}$ be a finite sample space, so that $\mathcal{M}_1(\mathcal{X})$ is isomorphic to the simplex of $\mathbb{R}^3$,
- → Admit that the objective function reaches its optimums on the extreme points.

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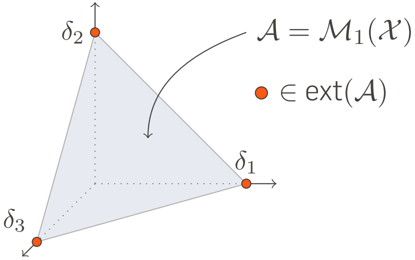

⇝ Extreme points are Dirac mass.

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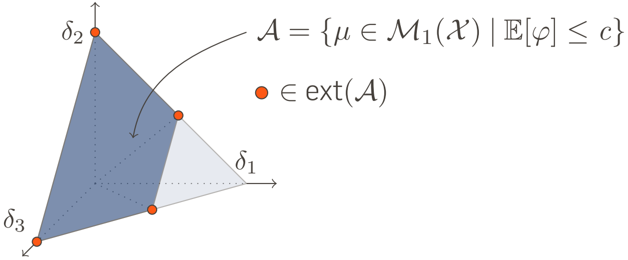

⇝ After adding **one** constraint, the extreme points are convex combination of at most **two** Dirac masses.

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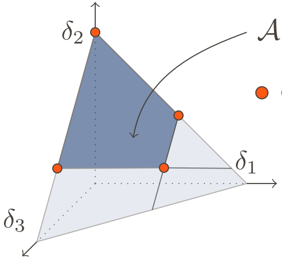

$$\mathcal{A} = \{\mu \in \mathcal{M}_1(\mathcal{X}) \mid \mathbb{E}[\varphi_1] \leq c_1, \mathbb{E}[\varphi_2] \leq c_2\}$$

● $\in \text{ext}(\mathcal{A})$

⇝ After adding **two** constraints, the extreme points are convex combination of at most **three** Dirac masses.

WINKLER'S CLASSIFICATION OF EXTREME POINTS

Heuristic

If you have N pieces of information relevant to the random variable X then it is enough to pretend that X takes at most $N+1$ values in $\mathcal{X}$.

1. Winkler (1988)

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Winkler theorem

The extreme measures of moment class

$$\{\mu \in \mathcal{M}_1(\mathcal{X}) \mid \mathbb{E}_\mu[\varphi_1] \leq 0, \ldots, \mathbb{E}_\mu[\varphi_n] \leq 0\}$$

are the discrete measures that are supported on at most $n+1$ points.

1. Winkler (1988)

SPACE REDUCTION

Let $\mathcal{A}$ be our multivariate optimization space

$$\mathcal{A} = \left\{ \mu = \otimes \mu_i \in \bigotimes_{i=1}^{p} \mathcal{M}_1([l_i, u_i]) \mid \mathbb{E}_{\mu_i}[x^j] \leq c_j^{(i)} \ , \ j = 1, \dots, N_i \right\} \ ,$$

$\rightsquigarrow$ Input i has N_i constraints.

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$$\longrightarrow \quad \mathcal{A}_\Delta = \left\{ \mu \in \mathcal{A} \mid \mu_i = \sum_{k=1}^{N_i+1} \omega_k^{(i)} \delta_{x_k}^{(i)} \right\}$$

OUQ REDUCTION THEOREM

OUQ reduction theorem

$$\begin{aligned}\inf_{\mu\in\mathcal{A}} F_\mu(h) &= \inf_{\mu\in\mathcal{A}} P_\mu(G(X)\leq h) = \inf_{\mu\in\mathcal{A}} \int \mathbb{1}_{\{G(x)\leq h\}} d\mu(x)\ ,\\ &= \inf_{\mu\in\mathcal{A}_\Delta} P_\mu(G(X)\leq h)\ ,\\ &= \inf_{\mu\in\mathcal{A}_\Delta} \sum_{i_1=1}^{N_1+1}\dots\sum_{i_p=1}^{N_p+1} \omega_{i_1}^{(1)}\dots\omega_{i_p}^{(p)}\ \mathbb{1}_{\{G(x_{i_1}^{(1)},\dots,x_{i_p}^{(p)})\leq h\}}\end{aligned}$$

→ The problem is now parameterized with the positions and the weights of the discrete measures

→ The code is evaluated on a grid of size $\prod_{i=1}^{p}(N_i+1)$

1. Owhadi et al. (2013)

DISCRETE MEASURES

Let enforce N equality constraint on a measure μ. OUQ theorem guaranties the solution 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

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

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

ADMISSIBLE MEASURE

We now possess a parameterization for our optimization problem. But generating a discrete measure having constraints on its moments is not easy...

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

$$\mathcal{A}_\Delta = \left\{ \mu = \sum_{i=1}^{3} \omega_i \delta_{x_i} \in \mathcal{M}_1([0,1]) \mid E_\mu[x] = 0.5,\ E_\mu[x^2] = 0.3 \right\} ,$$

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

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$$\rightsquigarrow \mu = \omega_1 \delta_{x_1} + \omega_2 \delta_{x_2} + \omega_3 \delta_{x_3}$$

$\mathbf{x} = (0.1, 0.4, 0.9)$ gives weights $\boldsymbol{\omega} = (0.05, 0.73, 0.22)$ ✓
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How to optimize over $\mathcal{A}_\Delta$?

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.

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↳ Canonical moments allows to efficiently explore the set of optimization $\mathcal{A}_\Delta$.

CANONICAL MOMENTS PARAMETERIZATION

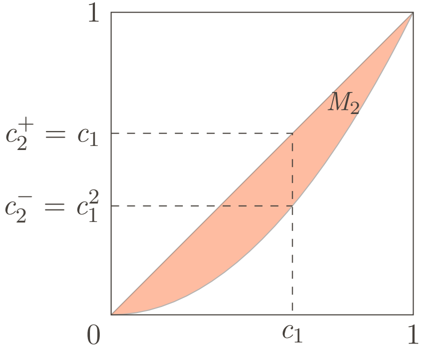
MOMENT SPACE

We define the moment space $M_n = \{\mathbf{c}_n(\mu) = (c_1, \ldots, c_n) \mid \mu \in \mathcal{M}_1([0,1])\}$

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 values of the $(n+1)$th moment a measure can have, when its moments up to order n equals to c_n.



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

- $p_n \in [0, 1]$,
- Canonical moments are defined up to degree $N = \min\{n \in \mathbb{N} \mid \mathbf{c}_n \in \partial M_n\}$ and $p_N \in \{0, 1\}$,
- The canonical moments are invariants by affine transformation. Which means we can always transform a measure supported on $[a, b]$ to $[0, 1]$

1. Dette, Studden (1997)

THE STIELTJES TRANSFORM

The Stieltjes transform is the analytic function on $\mathbb{C}\backslash\mathrm{supp}(\mu)$

$$S(z) = S(z,\mu) = \int_a^b \frac{d\mu(x)}{z-x}\ ,$$

If μ has a finite support : $S(z) = \sum_{i=1}^{n} \frac{\omega_i}{z-x_i} = \frac{Q_{n-1}(z)}{P_n^*(z)}\ ,$

$P_n^* = \prod_{i=1}^{n}(z-x_i) \rightsquigarrow$ its roots are the support points of μ

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Properties of the Stieltjes transform

P_n^* can be expressed recursively with the canonical moments :

$$P_{k+1}^*(x) = (x-a-(b-a)(\zeta_{2k}+\zeta_{2k+1}))P_k^*(x) - (b-a)^2\zeta_{2k-1}\zeta_{2k}P_{k-1}^*(x)$$

where $\zeta_k = (1-p_{k-1})p_k$

GENERATION OF ADMISSIBLE MEASURES

Theorem

Consider a sequence of moment $\mathbf{c}_n = (c_1, \dots, c_n) \in M_n$*, and the set of measure*

$$\mathcal{A}_\Delta = \left\{ \mu = \sum_{i=1}^{n+1} \omega_i \delta_{x_i} \in \mathcal{M}_1([a,b]) \mid \mathbb{E}_\mu(x^j) = c_j,\ j = 1, \dots, n \right\}.$$

We define

$$\Gamma = \left\{ (p_{n+1}, \dots, p_{2n+1}) \in [0,1]^{n+1} \mid p_i \in \{0,1\} \Rightarrow p_k = 0,\ k > i \right\}.$$

Then there exists a bijection between $\mathcal{A}_\Delta$ *and* Γ*.*

EFFECTIVE PARAMETERIZATION

Let $\mu \in \mathcal{A}_\Delta = \Big\{ \sum_{i=1}^{n+1} \omega_i \delta_{x_i} \in \mathcal{M}_1([a,b]) \mid \mathbb{E}_\mu(x^j) = c_j,\ j = 1, \ldots, n \Big\}$

EFFECTIVE PARAMETERIZATION

$$\mu \in \mathcal{A}_\Delta$$

$\downarrow$ The support of μ is the roots of a polynomial P^*_{n+1}

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$$(p_1, \dots, p_n, p_{n+1}, \dots, p_{2n+1})$$

EFFECTIVE PARAMETERIZATION

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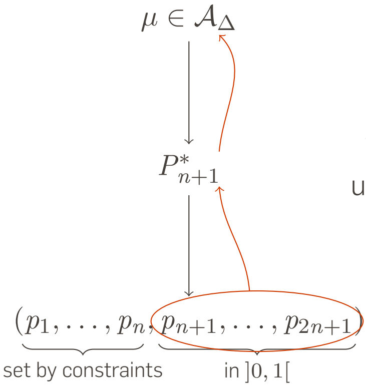
↓ Coefficients are defined with the sequence of canonical moments

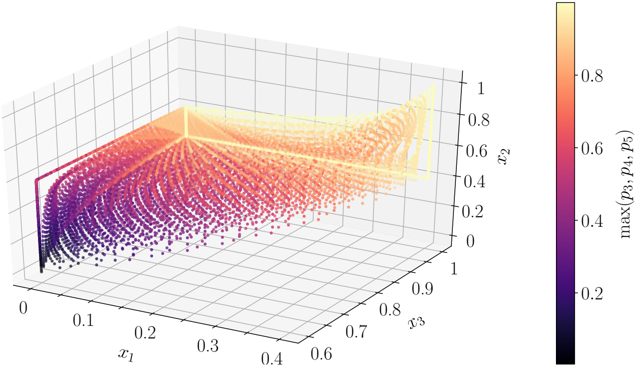
$$\big(\underbrace{p_1, \dots, p_n}_{\text{set by constraints}}, \underbrace{p_{n+1}, \dots, p_{2n+1}}_{\text{in }]0,1[}\big)$$

EFFECTIVE PARAMETERIZATION



We can explore the whole set $\mathcal{A}_\Delta$ using a parameterization in $]0,1[^{n+1}$.

SET OF ADMISSIBLE MEASURES



Each point correspond to a measure μ on $[0,1]$, we enforced $c_1 = 0.5$ and $c_2 = 0.3$ so that $p_1 = 0.5$ and $p_2 = 0.2$. We generated a regular grid where p_3, p_4 and p_5 goes from 0 to 1. The three Dirac masses corresponding to the roots of P_3^* are projected on each axis.

ALGORITHM - P.O.F CALCULATION

Inputs :

lower bounds, $\mathbf{l} = (l_1, \dots, l_p)$
upper bounds, $\mathbf{u} = (u_1, \dots, u_p)$
constraints sequences of moments, $\mathbf{c}_i = (c_1^{(i)}, \dots, c_{N_i}^{(i)})$ and its corresponding sequences of canonical moments, $\mathbf{p}_i = (p_1^{(i)}, \dots, p_{N_i}^{(i)})$ for $i = 1, \dots, p$

Ensure : $p_j^{(i)} \in [0, 1]$ for $j = 1, \dots, N_i$, $\quad i = 1, \dots, p$

1 : **function** P.O.F$(p_{N_1+1}^{(1)}, \dots, p_{2N_1+1}^{(1)}, \dots, p_{N_p+1}^{(p)}, \dots, p_{2N_p+1}^{(p)})$
2 : **for** $i = 1, \dots, p$ **do**
3 : **for** $k = 1, \dots N_i$ **do**
4 : $$P_{k+1}^{*(i)} = (X - l_i - (u_i - l_i)(\zeta_{2k}^{(i)} + \zeta_{2k+1}^{(i)}))P_k^{*(i)} - (u_i - l_i)^2 \zeta_{2k-1}^{(i)} \zeta_{2k}^{(i)} P_{k-1}^{*(i)}$$
5 : $x_1^{(i)}, \dots, x_{N_i+1}^{(i)} =$ roots$(P_{N_i+1}^{*(i)})$
6 : $\omega_1^{(i)}, \dots, \omega_{N_i+1}^{(i)} =$ weight$(x_1^{(i)}, \dots, x_{N_i+1}^{(i)}, \mathbf{c}_i)$
7 : **return** $\sum_{i_1=1}^{N_1+1} \dots \sum_{i_p=1}^{N_p+1} \omega_{i_1}^{(1)} \dots \omega_{i_p}^{(p)} \mathbb{1}_{\{G(x_{i_1}^{(1)}, \dots, x_{i_p}^{(p)}) \le h\}}$

APPLICATIONS

PRESENTATION OF THE TOY CASE

	Distribution	Bounds	Mean	2nd moment	3rd moment
Q	$Gumbel(1013, 558)$	$[160, 3580]$	1320.42	2.1632 e6	4.18 e9
K_s	$\mathcal{N}(\overline{x} = 30, \sigma = 7.5)$	$[12.55, 47.45]$	30	949	31422
Z_v	$\mathcal{U}(49, 51)$	$[49, 51]$	50	2500	125050
Z_m	$\mathcal{U}(54, 55)$	$[54, 55]$	54.5	2970	161892

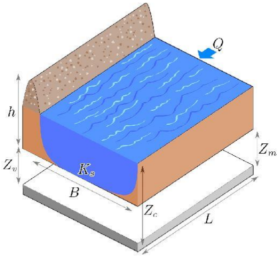


Figure : Hydraulic model.

$$H = \left(\frac{Q}{300 K_s \sqrt{\frac{Z_m - Z_v}{5000}}} \right)^{3/5}$$

COMPARAISON OF DIFFERENTS MOMENTS CONSTRAINTS

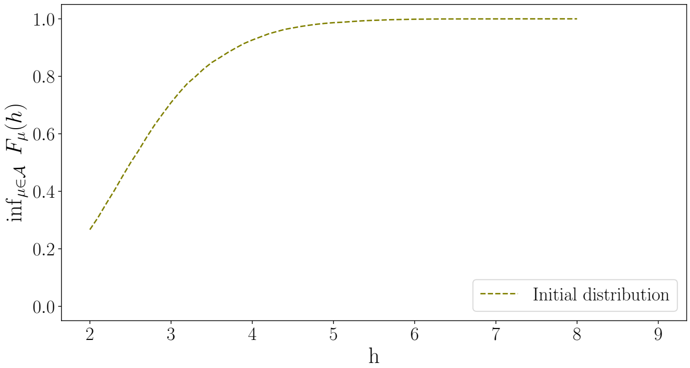


Figure : The more we add constraints, the more the space size is reduced, hence the minimum obtained is higher.

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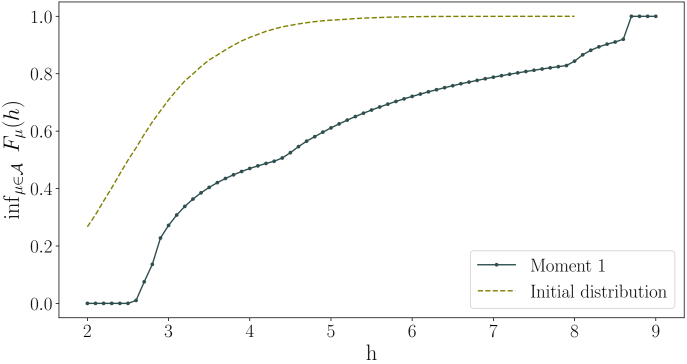

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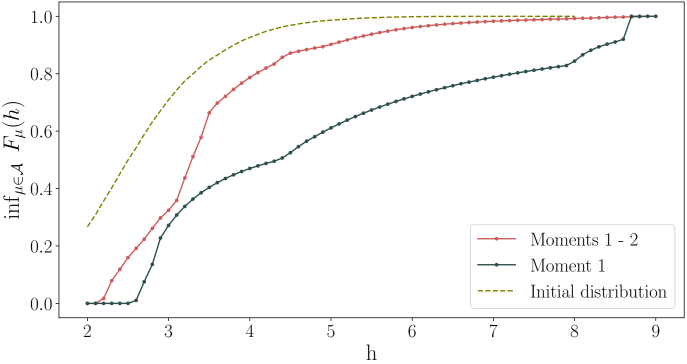

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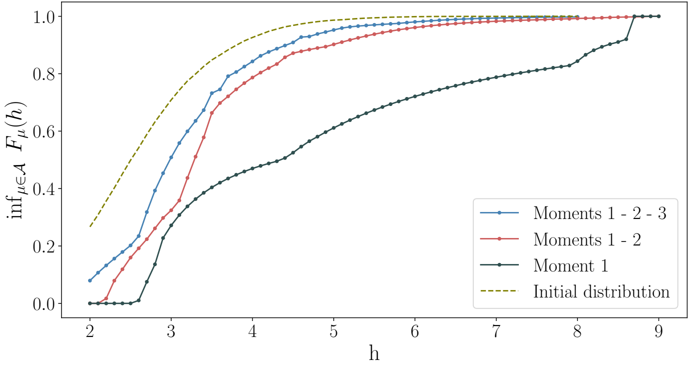

Figure : The more we add constraints, the more the space size is reduced, hence the minimum obtained is higher.

PRESENTATION OF THE USE-CASE

Our use-case is a thermal-hydraulic computer experiment, which simulates a Intermediate Break Loss Of Coolant Accident (IBLOCA). The variable of interest is the maximum temperature.

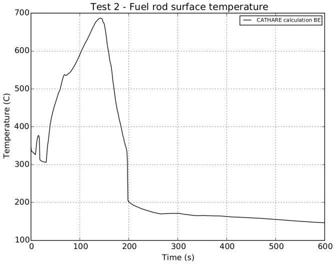

Figure : CATHARE temperature output for nominal parameters.

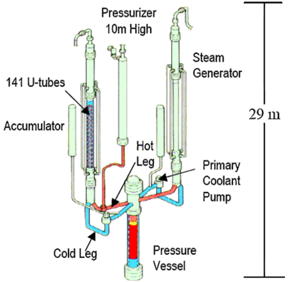

Figure : The replica of a water pressured reactor, with the hot and cold leg.

PRESENTATION OF THE USE-CASE

The code takes 27 inputs, but using a screening strategy we highlighted the 9 most influent variables.

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.

COMPARAISON WITH THE MYSTIC FRAMEWORK

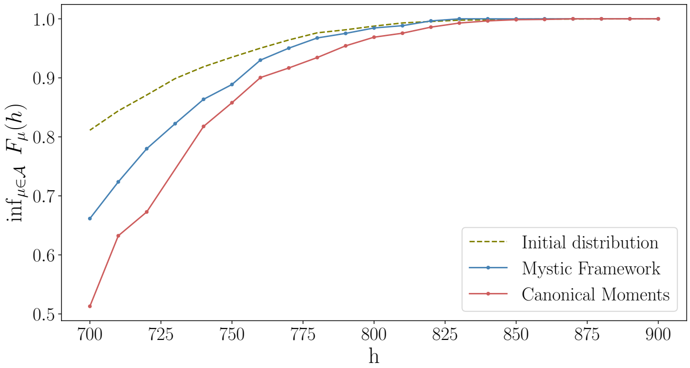

Figure : Our algorithm performs better than existing solution. Mystic Framework struggles to explore the whole optimization space.

FURTHER WORKS

- Different optimization spaces :

	All distributions	Unimodal distributions
Constraints	Moment constraints $\mathbb{E}_\mu[x^j] \leqq c_j$	Moment constraints $\mathbb{E}_\mu[x^j] \leqq c_j$
Extreme points	$\mu = \sum \omega_i \delta_{x_i}$	$\mu = \sum \omega_i \mathbf{u}_{z_i}$

- Different quantities of interest :
  - → Superquantile.
  - → Bayesian estimate associated to a given utility or loss function.

CONCLUSION

- → We optimize a measure affine functional on the extreme point of the moment class.
- → The extreme points are discrete measures. Canonical moments provide an efficient way to explore the set of extreme points
- → Global optimization free of constraints is performed, achievable up to dimension 10, due to exponential growing cost.

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THANK YOU FOR YOUR ATTENTION !