Monte Carlo Simulation

with Imprecise Random Variables

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IPW2015, Liverpool, UK

Problem statement and outline of presentation

Given

• Expensive input-output map $g : \mathbb{R}^n \to \mathbb{R} : x \to g(x)$.

E.g. finite element computations (minutes or hours per computation).

• Family $\{X_{\lambda}\}_{\lambda \in \Lambda}$ of random variables modelling the uncertainty of variable *x*.

Aim

- Upper/lower probabilities that $g(x) \in B$.
- Upper/lower probabilities that $g(x) \le y$. (upper/lower cumulative distribution function, p-box)
- Upper/lower probabilities that $g(x) \le 0$. (upper/lower probability of failure)

Two approaches

- Monte-Carlo simulation of the family $\{g(X_{\lambda})\}_{\lambda \in \Lambda}$.
- Monte-Carlo simulation of the random set X generated by {g(X_λ)}_{λ∈Λ}.

Numerical example

• The efficiency of the two approaches is demonstrated by means of a moderate scale engineering structure (simplified model of ARIANE 5 front skirt).

Two approaches

1 Family $\{X_{\lambda}\}_{\lambda \in \Lambda}$ of random variables

- Probability space (Ω, Σ, m) .
- Family $\{X_{\lambda}\}_{\lambda \in \Lambda}$ of random variables

 $X_{\lambda}: \Omega \to \mathbb{R}: \omega \to X_{\lambda}(\omega).$

• Probability $P(X_{\lambda} \in B)$ for fixed λ :

$$P(X_{\lambda} \in B) = \int_{\Omega} \mathbb{1}_{X_{\lambda}(\omega) \in B} \, \mathrm{d}m(\omega).$$

(for initial analysis we drop the map g)

2 Random set \mathfrak{X} based on $\{X_{\lambda}\}_{\lambda \in \Lambda}$

• Set-valued map $\mathfrak{X}:\Omega\to\mathbb{R}$ defined by

$$\mathfrak{X}(\boldsymbol{\omega}) = \{ X_{\boldsymbol{\lambda}}(\boldsymbol{\omega}) : \boldsymbol{\lambda} \in \boldsymbol{\Lambda} \}.$$

(focal set at fixed ω)

• $\boldsymbol{\mathfrak{X}}$ is a random set, with upper/lower inverses

$$\begin{aligned} \mathfrak{X}^{-}(B) &= \{ \boldsymbol{\omega} \in \Omega : \mathfrak{X}(\boldsymbol{\omega}) \cap B \neq \emptyset \}, \\ \mathfrak{X}_{-}(B) &= \{ \boldsymbol{\omega} \in \Omega : \mathfrak{X}(\boldsymbol{\omega}) \subseteq B \}. \end{aligned}$$

Two approaches

1 Family $\{X_{\lambda}\}_{\lambda \in \Lambda}$ of random variables	2 Random set \mathfrak{X} based on $\{X_{\lambda}\}_{\lambda \in \Lambda}$		
• Probability space (Ω, Σ, m) .	 Set-valued map X : Ω → ℝ defined by X(ω) = {X_λ(ω) : λ ∈ Λ}. (focal set at fixed ω) X is a random set, with upper/lower 		
• Family $\{X_{\lambda}\}_{\lambda \in \Lambda}$ of random variables			
$X_{\boldsymbol{\lambda}}: \Omega \to \mathbb{R}: \boldsymbol{\omega} \to X_{\boldsymbol{\lambda}}(\boldsymbol{\omega}).$			
• Probability $P(X_{\lambda} \in B)$ for fixed λ :			
$P(X_{\lambda} \in B) = \int_{\Omega} \mathbb{1}_{X_{\lambda}(\boldsymbol{\omega}) \in B} \mathrm{d}m(\boldsymbol{\omega}).$	Inverses		
522	$\mathfrak{X}^{-}(B) = \{ \boldsymbol{\omega} \in \Omega : \mathfrak{X}(\boldsymbol{\omega}) \cap B \neq \boldsymbol{\varnothing} \},$		
(for initial analysis we drop the map g)	$\mathcal{X}_{-}(B) = \{ \omega \in \Omega : \mathcal{X}(\omega) \subseteq B \}.$		
Lower/upper probabilities for $\{X_{oldsymbol{\lambda}}\}_{oldsymbol{\lambda}\in \Lambda}$	Lower/upper probabilities for ${\mathfrak X}$		
$\underline{P}(B) = \inf_{\lambda \in \Lambda} P(X_{\lambda} \in B) = \inf_{\lambda \in \Lambda} \int_{\Omega} \mathbb{1}_{X_{\lambda}(\omega) \in B} \mathrm{d}m(\omega)$	$\underline{P}(B) = m(\mathfrak{X}_{-}(B)) = \int_{\Omega} \mathbb{1}_{\mathfrak{X}(\omega) \subseteq B} \mathrm{d}m(\omega)$		
$\overline{P}(B) = \sup_{\lambda \in \Lambda} P(X_{\lambda} \in B) = \sup_{\lambda \in \Lambda} \int_{\Omega} \mathbb{1}_{X_{\lambda}(\omega) \in B} \mathrm{d}m(\omega)$	$\widetilde{P}(B) = m(\mathfrak{X}^{-}(B)) = \int_{\Omega} \mathbb{1}_{\mathfrak{X}(\boldsymbol{\omega}) \cap B \neq \varnothing} \mathrm{d}m(\boldsymbol{\omega})$		

Two approaches

1 Family $\{X_{\lambda}\}_{\lambda\in\Lambda}$ of random variables	2 Random set \mathfrak{X} based on $\{X_{\lambda}\}_{\lambda \in \Lambda}$	
 Probability space (Ω, Σ, m). Family {X_λ}_{λ∈Λ} of random variables X_λ : Ω → ℝ : ω → X_λ(ω). Probability P(X_λ ∈ B) for fixed λ: P(X_λ ∈ B) = ∫_Ω 1_{X_λ(ω)∈B} dm(ω). (for initial analysis we drop the map g) 	 Set-valued map X : Ω → ℝ defined by X(ω) = {X_λ(ω) : λ ∈ Λ}. (focal set at fixed ω) X is a random set, with upper/lower inverses X⁻(B) = {ω ∈ Ω : X(ω) ∩ B ≠ ∅}, X₋(B) = {ω ∈ Ω : X(ω) ⊆ B}. 	
Lower/upper probabilities for $\{X_{m{\lambda}}\}_{m{\lambda}\in\Lambda}$	Lower/upper probabilities for ${\mathfrak X}$	
$\underline{P}(B) = \inf_{\lambda \in \Lambda} P(X_{\lambda} \in B) = \inf_{\lambda \in \Lambda} \int_{\Omega} \mathbb{1}_{X_{\lambda}(\omega) \in B} \mathrm{d}m(\omega)$ $\overline{P}(B) = \sup_{\lambda \in \Lambda} P(X_{\lambda} \in B) = \sup_{\lambda \in \Lambda} \int_{\Omega} \mathbb{1}_{X_{\lambda}(\omega) \in B} \mathrm{d}m(\omega)$	$ \underbrace{\mathcal{P}(B) = m(\mathfrak{X}_{-}(B)) = \int_{\Omega} \mathbb{1}_{\mathfrak{X}(\omega) \subseteq B} \mathrm{d}m(\omega)}_{\widetilde{P}(B) = m(\mathfrak{X}^{-}(B)) = \int_{\Omega} \mathbb{1}_{\mathfrak{X}(\omega) \cap B \neq \emptyset} \mathrm{d}m(\omega)} $	
Theorem		

Simulation of a family $\{X_{\lambda}\}_{\lambda \in \Lambda}$ of random variables

1 Basic sample $x_1, \ldots, x_{N_{samp}}$

- Generate a sample $x_1, \ldots, x_{N_{samp}}$ which is distributed as a **basic random variable** X_* .
- Distribution of X_* should cover a greater range than a distribution of a single X_{λ} does.

2 N_{samp} function evaluations $g(x_k), k = 1, \dots, N_{\text{samp}}$

• We compute $g(x_k)$ either using g directly or a cost saving surrogate model \tilde{g} .

3 Approximation of $P(g(X_{\lambda}) \leq y)$

- Probability $P(g(X_{\lambda}) \leq y)$ for fixed λ is computed by **reweighting** the original sample.
- Weights w_k(λ) depending on parameters λ for reweighting the sample x₁,...,x<sub>N_{samp} according to the distribution of X_λ (cf. importance sampling):
 </sub>

$$w_k(\lambda) = \frac{f_{X_{\lambda}}(x_k)}{f_{X_*}(x_k)} \frac{1}{N_{\mathsf{samp}}} = \frac{f_{\mathsf{new}}(x_k)}{f_{\mathsf{old}}(x_k)} \frac{1}{N_{\mathsf{samp}}}$$

• Obtaining $P(g(X_{\lambda}) \leq y)$ for different X_{λ} without additional function evaluations of g:

$$P(g(X_{\lambda}) \leq y) = \int_{\Omega} \mathbb{1}_{g(X_{\lambda}(\omega)) \leq y} \, \mathrm{d}m(\omega) \approx \sum_{k=1}^{N_{\mathrm{samp}}} \mathbb{1}_{g(X_{\lambda}(\omega_{k})) \leq y} \cdot w_{k}(\lambda) = \sum_{k=1}^{N_{\mathrm{samp}}} \mathbb{1}_{g(x_{k}) \leq y} \cdot w_{k}(\lambda).$$

Simulation of a family $\{X_{\lambda}\}_{\lambda \in \Lambda}$ of random variables

- 4 Approximation of upper/lower cumulative distribution functions $\overline{F}(y)$ and $\underline{F}(y)$
- We have to solve the following global optimization problems:

$$\begin{split} \overline{F}(\mathbf{y}) &= \overline{P}(g \leq \mathbf{y}) = \sup_{\boldsymbol{\lambda} \in \Lambda} P(g(X_{\boldsymbol{\lambda}}) \leq \mathbf{y}) \approx \max_{\boldsymbol{\lambda} \in \Lambda} \sum_{k=1}^{N_{\text{samp}}} \mathbbm{1}_{g(x_k) \leq \mathbf{y}} \cdot w_k(\boldsymbol{\lambda}) = \max_{\boldsymbol{\lambda} \in \Lambda} p(\boldsymbol{\lambda}), \\ \underline{F}(\mathbf{y}) &= \underline{P}(g \leq \mathbf{y}) = \inf_{\boldsymbol{\lambda} \in \Lambda} P(g(X_{\boldsymbol{\lambda}}) \leq \mathbf{y}) \approx \min_{\boldsymbol{\lambda} \in \Lambda} \sum_{k=1}^{N_{\text{samp}}} \mathbbm{1}_{g(x_k) \leq \mathbf{y}} \cdot w_k(\boldsymbol{\lambda}) = \min_{\boldsymbol{\lambda} \in \Lambda} p(\boldsymbol{\lambda}). \end{split}$$

• Smooth and cheap objective function for fixed y: $p(\lambda) = \sum_{k=1}^{N_{samp}} \mathbb{1}_{g(x_k) \le y} \cdot w_k(\lambda).$

- Standard optimization algorithms can be applied because of the smoothness of $p(\lambda)$.
- Effort: N_{obj} · N_{samp} reweightings, N_{samp} expensive function evaluations of g.
- Remark: Different samples $x_1(\lambda), \ldots, x_{N_{samp}}(\lambda)$ for different $\lambda \in \Lambda$ would lead to a non-smooth objective function

$$q(\lambda) = \sum_{k=1}^{N_{\mathsf{samp}}} \mathbbm{1}_{g(x_k(\lambda)) \leq y} \cdot \frac{1}{N_{\mathsf{samp}}}.$$



Simulation of a random set $\boldsymbol{\mathcal{X}}$

1 Propagation of a random set through g

- $\mathfrak{G}(\boldsymbol{\omega}) = g(\mathfrak{X}(\boldsymbol{\omega})) = \{g(X_{\boldsymbol{\lambda}}(\boldsymbol{\omega}))) : \boldsymbol{\lambda} \in \boldsymbol{\Lambda}\}$
- $\mathfrak{G}(\boldsymbol{\omega}) = [\underline{\mathfrak{G}}(\boldsymbol{\omega}), \overline{\mathfrak{G}}(\boldsymbol{\omega})]$ random interval

•
$$\underline{G}(\boldsymbol{\omega}) = \min g(\mathfrak{X}(\boldsymbol{\omega})), \ \overline{G}(\boldsymbol{\omega}) = \max g(\mathfrak{X}(\boldsymbol{\omega}))$$

2 Cumulative distribution functions

•
$$\widetilde{F}(y) = \widetilde{P}(g \le y), \ \ \widetilde{F}(y) = \widetilde{P}(g \le y)$$

•
$$\widetilde{F}(y) = P((-\infty, y] \cap [\underline{\mathcal{G}}, \overline{\mathcal{G}}] \neq \emptyset) = P(\underline{\mathcal{G}} \leq y) = F_{\underline{\mathcal{G}}}(y)$$

•
$$\underline{F}(y) = P([\underline{G}, \overline{G}] \subset (-\infty, y]) = P(\overline{G} \leq y) = F_{\overline{G}}(y)$$

3 Algorithm for computing $\widetilde{F}(y)$

Generate ω₁,..., ω_{Nsamp} distributed as m.

• For each ω_k , estimate $\underline{G}(\omega_k) \approx \min g(X_{\lambda_i}(\omega_k))$ using grid points $\lambda_1, \dots, \lambda_{N_{\text{grid}}}$ on Λ .

•
$$\widetilde{F}(y) \approx \sum_{k=1}^{N_{\text{samp}}} \mathbb{1}_{\underline{\mathcal{G}}(\omega_k) \leq y} \cdot \frac{1}{N_{\text{samp}}}.$$

Effort: $N_{\text{grid}} \cdot N_{\text{samp}}$ expensive evaluations of g.

4 Cost saving methods, approximation of g by surrogate models \tilde{g}_i

Starting point: Collocation points x_j , $j = 1, ..., N_{coll}$, in \mathbb{R}^n and N_{coll} evaluations $y_j = g(x_j)$.

Stochastic surrogate models \widetilde{g}_i of maps $\Omega \to g \circ X_{\lambda_i}$:

- Collocation points x_j are pulled back to probability space Ω , i.e., for each λ_i and x_j , a collocation point $\omega_{ij} = X_{\lambda_i}^{-1}(x_j)$ in Ω is computed.
- Clearly, $y_j = g(X_{\lambda_i}(\boldsymbol{\omega}_{ij})) = g(x_j)$ for every *i*.
- Stochastic surrogate models *g̃_i*, *i* = 1,...,N_{grid}, are obtained by regression through the data points (ω_{ij}, y_j), *j* = 1,...,N_{coll}.
- Finally, one computes $\underline{G}(\boldsymbol{\omega}) \approx \min_{i=1,\dots,N_{\text{grid}}} \widetilde{g}_i(\boldsymbol{\omega})$.
- Based on a sample $\omega_1, \ldots, \omega_{N_{coll}}$, a Monte Carlo sample of \underline{G} is obtained.

Effort: N_{coll} expensive evaluations of g;

 N_{grid} linear regressions (moderate cost);

 N_{samp} cheap evaluations of \tilde{g}_i for each *i*.

Advantage of stochastic surrogate models \tilde{g}_i on Ω :

- Use of orthogonal polynomials with respect to the measure *m*.
- In the Gaussian case, Ω is standard Gaussian space of dimension n×(polynomial order) and X⁻¹_{λi}(x_j) is simply (x_j - μ_i)/σ_i (in each component of x_j).

Numerical example: simplified model of ARIANE 5 front skirt

Limit state function:

- $g(x) = 1 \max\{\mathsf{PEEQ}(x)/0.07, \mathsf{SP}(x)/155\}$
- PEEQ: maximum value of equivalent plastic strain.
- SP: maximum principal stress.

Parameters:

sphere 2

cylinder 3

cylinder 2

cylinder 1

- 35 parameters in total.
- We model the uncertainty of the 3 most significant parameters using families {X_{(μi,σi}}} of Gaussian random variables.

	description	μ_i	σ_i^2
x_1 x_2	yield stress in cylinder 3 pressures loads in sphere 2	[350, 375] N/mm ² [0.38, 0.41] N/mm ²	[0.01, 0.02] [0.01, 0.02]
<i>x</i> ₃	temperature loads in cylinder 1	[430, 470] K	[0.01, 0.02]

- The random variables are independent.
- Family $\{X_{\lambda}\}_{\lambda \in \Lambda}$ of joint random variables, $\lambda = (\mu_1, \mu_2, \mu_3, \sigma_1^2, \sigma_2^2, \sigma_3^2)$ $\Lambda = [350, 375] \times [0.38, 0.41] \times [430, 470] \times [0.01, 0.02] \times [0.01, 0.02] \times [0.01, 0.02].$

Numerical example: results



Conclusion

Two interpretations of imprecise probability models

- (1) Information given by a family $\{g(X_{\lambda})\}_{\lambda \in \Lambda}$.
- (2) Information given by the random set \mathcal{X} generated by the family.

Two numerical methods

- (1) Reweighting a basic sample.
- (2) Fitting stochastic surrogate models to all $g(X_{\lambda})$.

Optimization

(1) and (2).

Numerical effort

(1) < (2).

Choice of the method

Depends on interpretation of imprecise model.