

Imprecise random variables, random sets, and Monte Carlo simulation

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Problem

Given

- Expensive input-output map $g : \mathbb{R}^n \rightarrow \mathbb{R} : x \rightarrow g(x)$.
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 $g(x) \leq y$ (upper/lower cumulative distribution functions).
- Upper/lower probabilities that $g(x) \leq 0$ (**upper/lower probability of failure**).

Two approaches

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

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

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

- Probability $P(X_\lambda \in B)$ for fixed X_λ :

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

(for initial analysis we drop the map g)

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

- Set-valued map $\mathcal{X} : \Omega \rightarrow \mathbb{R}$ defined by

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

- \mathcal{X} is a random set, if upper/lower inverses

$$\mathcal{X}^-(B) = \{\omega \in \Omega : \mathcal{X}(\omega) \cap B \neq \emptyset\},$$

$$\mathcal{X}_-(B) = \{\omega \in \Omega : \mathcal{X}(\omega) \subseteq B\}$$

are measurable subsets of Ω .

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Lower/upper probabilities for $\{X_\lambda\}_{\lambda \in \Lambda}$

$$\underline{P}(B) = \inf_{\lambda \in \Lambda} P(X_\lambda \in B) = \inf_{\lambda \in \Lambda} \int_{\Omega} \mathbb{1}_{X_\lambda(\omega) \in B} dm(\omega)$$

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Lower/upper probabilities for \mathcal{X}

$$\underline{P}(B) = m(\mathcal{X}_-(B)) = \int_{\Omega} \mathbb{1}_{\mathcal{X}(\omega) \subseteq B} dm(\omega)$$

$$\tilde{P}(B) = m(\mathcal{X}^-(B)) = \int_{\Omega} \mathbb{1}_{\mathcal{X}(\omega) \cap B \neq \emptyset} dm(\omega)$$

Two approaches

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

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

- Probability $P(X_\lambda \in B)$ for fixed X_λ :

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Lower/upper probabilities for \mathcal{X}

$$\underline{P}(B) = m(\mathcal{X}_-(B)) = \int_{\Omega} \mathbb{1}_{\mathcal{X}(\omega) \subseteq B} dm(\omega)$$

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Theorem

$$\underline{\tilde{P}} \leq \underline{P} \leq \bar{P} \leq \tilde{P}$$

\mathcal{X} is more imprecise than $\{X_\lambda\}_{\lambda \in \Lambda}$!

Example

- Probability space: $(\Omega, \Sigma, m) = (\mathbb{R}, \mathcal{B}(\mathbb{R}), m)$, $m(B) = \int_{\mathbb{R}} \mathbb{1}_{\omega \in B} \frac{1}{\sqrt{2\pi}} e^{-\omega^2/2} d\omega$.
- Family $\{X_{(\mu, \sigma)}\}_{(\mu, \sigma) \in \Lambda}$: $X_{(\mu, \sigma)}(\omega) = \sigma\omega + \mu \implies X_{(\mu, \sigma)} \sim \mathcal{N}(\mu, \sigma^2)$.
- $\Lambda = [\underline{\mu}, \bar{\mu}] \times [\underline{\sigma}, \bar{\sigma}] = [-0.5, 2] \times [1, 2]$, $B = [1, 2.5]$.

$$\mathcal{X}(\omega) = \{X_{\lambda}(\omega) : \lambda \in \Lambda\} = [\underline{\mathcal{X}}(\omega), \bar{\mathcal{X}}(\omega)]$$

$$\underline{\mathcal{X}}(\omega) = \inf_{\substack{\mu \in [\underline{\mu}, \bar{\mu}] \\ \sigma \in [\underline{\sigma}, \bar{\sigma}]}} X_{(\mu, \sigma)}(\omega) = \begin{cases} \bar{\sigma}\omega + \underline{\mu} & \omega < 0 \\ \underline{\sigma}\omega + \underline{\mu} & \omega \geq 0 \end{cases}$$

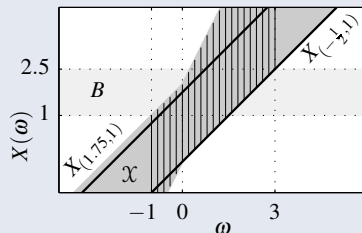
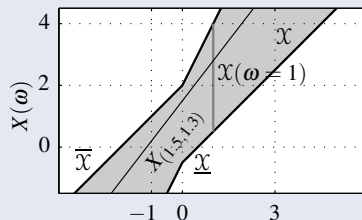
$$\bar{\mathcal{X}}(\omega) = \sup_{\substack{\mu \in [\underline{\mu}, \bar{\mu}] \\ \sigma \in [\underline{\sigma}, \bar{\sigma}]}} X_{(\mu, \sigma)}(\omega) = \begin{cases} \underline{\sigma}\omega + \bar{\mu} & \omega < 0 \\ \bar{\sigma}\omega + \bar{\mu} & \omega \geq 0 \end{cases}$$

$$\underline{P}(B) = \inf_{(\mu, \sigma) \in \Lambda} P(X_{(\mu, \sigma)} \in B) = P(X_{(-0.5, 1)} \in B) = 0.0655$$

$$\bar{P}(B) = \sup_{(\mu, \sigma) \in \Lambda} P(X_{(\mu, \sigma)} \in B) = P(X_{(1.75, 1)} \in B) = 0.5467$$

$$P(B) = m(\mathcal{X}_-(B)) = m(\emptyset) = 0.0000$$

$$\begin{aligned} \tilde{P}(B) &= m(\mathcal{X}^-(B)) = m([-1, 3]) \\ &= \Phi(3) - \Phi(-1) = 0.8400 \end{aligned}$$



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

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

- Generate a sample $x_1, \dots, x_{N_{\text{samp}}}$ 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 $w_k(\lambda)$ depending on parameters λ for reweighting the sample $x_1, \dots, x_{N_{\text{samp}}}$ according to the distribution of X_λ :

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

where f_{X_λ} and f_{X_*} are strictly positive densities.

- $P(g(X_\lambda) \leq y)$ for different X_λ **without additional function evaluations** of g :

$$P(g(X_\lambda) \leq y) = \int_{\Omega} \mathbb{1}_{g(X_\lambda(\omega)) \leq y} \, d\mathbf{m}(\omega) \approx \sum_{k=1}^{N_{\text{samp}}} \mathbb{1}_{g(X_\lambda(\omega_k)) \leq y} \cdot w_k(\lambda) = \sum_{k=1}^{N_{\text{samp}}} \mathbb{1}_{g(x_k) \leq y} \cdot w_k(\lambda).$$

4 Approximation of $\bar{P}(g \leq y)$ and $\underline{P}(g \leq y)$

For the computation of the upper/lower probabilities $\bar{P}(g \leq y)$ and $\underline{P}(g \leq y)$ we

- use a grid of representative parameter values λ_i ,
- estimate the probabilities $P(g(X_{\lambda_i}) \leq y)$ at the grid points λ_i by means of MC simulation
- and take the maximum/minimum value:

$$\bar{P}(g \leq y) = \sup_{\lambda \in \Lambda} P(g(X_\lambda) \leq y) \approx \max_{i=1, \dots, N_{\text{grid}}} P(g(X_{\lambda_i}) \leq y) \approx \max_{i=1, \dots, N_{\text{grid}}} \sum_{k=1}^{N_{\text{samp}}} \mathbb{1}_{g(x_k) \leq y} \cdot w_k(\lambda_i),$$

$$\underline{P}(g \leq y) \approx \min_{i=1, \dots, N_{\text{grid}}} \sum_{k=1}^{N_{\text{samp}}} \mathbb{1}_{g(x_k) \leq y} \cdot w_k(\lambda_i).$$

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

1 Propagation of a random set through g

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

2 Cumulative distribution functions

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

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

- Generate $\omega_1, \dots, \omega_{N_{\text{samp}}}$ distributed as m .
- For each ω_n , estimate $\underline{\mathcal{G}}(\omega_n) \approx \min_i g(X_{\lambda_i}(\omega_n))$ using grid points $\lambda_1, \dots, \lambda_{N_{\text{grid}}}$ on Λ .
- $\overline{F}(y) \approx \sum_{k=1}^{N_{\text{samp}}} \mathbb{1}_{\underline{\mathcal{G}}(\omega_k) \leq 0} \cdot \frac{1}{N_{\text{samp}}}$.

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

4 Cost saving methods, approximation of g by a **surrogate model** \tilde{g}

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

Two levels are at hand: $\Omega \xrightarrow{X_\lambda} \mathbb{R}^n \xrightarrow{g} \mathbb{R}$.

(A) **Surrogate model \tilde{g} of the map $g : \mathbb{R}^n \rightarrow \mathbb{R}$:**

To obtain the lower bound \underline{g} we replace g by \tilde{g} : $\underline{g}(\omega_n) \approx \min_{i=1, \dots, N_{\text{grid}}} \tilde{g}(X_{\lambda_i}(\omega_n))$.

Effort: One surrogate model \tilde{g} ,

$N_{\text{grid}} \cdot N_{\text{samp}}$ cheap evaluations of \tilde{g} and N_{coll} expensive evaluations of g .

(B) **Surrogate models \tilde{g}_i of maps $\Omega \rightarrow g \circ X_{\lambda_i}$:**

- Collocation points x_j are pulled back to Ω .
- For each λ_i and x_j , we get a collocation point $\omega_{ij} = X_{\lambda_i}^{-1}(x_j)$ in Ω .
- Clearly, $y_j = g(X_{\lambda_i}(\omega_{ij})) = g(x_j)$ for every i . Then $\underline{g}(\omega_n) \approx \min_{i=1, \dots, N_{\text{grid}}} \tilde{g}_i(\omega_n)$.

Effort: N_{grid} surrogate models \tilde{g}_i ,



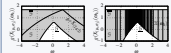
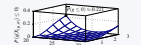
N_{samp} cheap evaluations of \tilde{g}_i for each i and N_{coll} expensive evaluations of g .

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

- Use of orthogonal polynomials with respect to the measure m .
- In the Gaussian case it means Hermite expansion.

Please visit our poster for more details and numerical examples!

Thank you for your attention!

<p>Problem</p> <p>Expressive input-output map $\mu: \mathbb{S}^n \rightarrow \mathbb{R}$, $\mu(x) = g(x)$ and family $\{X_{i, \omega}\}_{i \in I}$ of random variables.</p> <p>Given: Expressive random variables that $\mu(x) = g(x)$ at all points x of a bounded domain $\Omega \subseteq \mathbb{R}^n$.</p> <p>Method: Monte-Carlo simulation of μ by random set $\tilde{\mu}$ generated by $\{X_{i, \omega}\}_{i \in I}$.</p> <p>Family $\{X_{i, \omega}\}_{i \in I}$ of random variables</p> <ul style="list-style-type: none"> Probability space $(\Omega, \mathcal{L}, \mathbb{P})$. Family $\{X_{i, \omega}\}_{i \in I}$ of random variables $X_i: \Omega \rightarrow \mathbb{R}$, $i \in I$. Probability $P(X_i \in A)$ for fixed X_i: $P(X_i \in A) = \int_{\omega \in \Omega: X_i(\omega) \in A} d\mathbb{P}(\omega)$ (the total surface area of the map μ). <p>Lower upper probabilities for $\{X_{i, \omega}\}_{i \in I}$</p> <p>$\underline{P}(X_i \in A) = \inf_{\omega \in \Omega} P(X_i(\omega) \in A)$ $\overline{P}(X_i \in A) = \sup_{\omega \in \Omega} P(X_i(\omega) \in A)$</p> <p>Upper lower probabilities for $\{X_{i, \omega}\}_{i \in I}$</p> <p>$\underline{P}(X_i \in A) = \inf_{\omega \in \Omega} P(X_i(\omega) \in A)$ $\overline{P}(X_i \in A) = \sup_{\omega \in \Omega} P(X_i(\omega) \in A)$</p>	<p>Example</p> <ul style="list-style-type: none"> Probability space: $(\Omega, \mathcal{L}, \mathbb{P})$, $\omega \in \Omega = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}} dt$. Family $\{X_{i, \omega}\}_{i \in I}$ of random variables: $X_i: \Omega \rightarrow \mathbb{R}$, $i \in I$. $\mathbb{P}(X_i \in A) = \int_{\omega \in \Omega: X_i(\omega) \in A} d\mathbb{P}(\omega)$. $\mathbb{P}(X_i \in A) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}} dt$, $A = [a, b]$, $a < b$. 
<p>Assumption: $\mu: \mathbb{S}^n \rightarrow \mathbb{R}$ is a continuous function. A is a compact subset of an affine space and the map $\mu: \mathbb{S}^n \rightarrow \mathbb{R}$ and continuous for each fixed $\omega \in \Omega$.</p> 	<p>Example: Beam loaded on spring with uncertain spring constant</p> <ul style="list-style-type: none"> Given: Limit state function μ and $\{X_{i, \omega}\}_{i \in I}$ for spring constant κ as in the above example, but here with $A = \{x \in \mathbb{R}^n: \mu(x) \leq 0\}$. Goal: Upper/lower probabilities of failure. <p>Simulation of a random set</p> <ul style="list-style-type: none"> Grid points $\{x_j\}_{j=1, \dots, N}$ with $x_j = (-20, 21, \dots, 30)$ and $\omega_j = 0.5, 1.5, \dots, 3$ on set $A = \{x \in \mathbb{R}^n: \mu(x) \leq 0\}$. Focal set $\tilde{\mu}$ of the random set $\tilde{\mu}$ is approximated by $\tilde{\mu} = \bigcup_{j=1, \dots, N} \{x_j\}$. Approximation of the upper probability of failure of the beam by means of Monte Carlo simulation: $\overline{P}(\mu \leq 0) = \overline{P}(\tilde{\mu} \leq 0) = \frac{1}{N} \sum_{j=1, \dots, N} \mathbb{1}_{\{x_j \in A\}}$
<p>Simulation of a family of random variables</p> <p>Goal: Approximation of $\mu(x) \in \tilde{\mu}$ by means of Monte Carlo simulation using only one sample for all random variables X_i, $i \in I$.</p> <p>1. Basic sample x_1, \dots, x_N</p> <ul style="list-style-type: none"> We generate a sample x_1, \dots, x_N which distributed as a basic random variable X_i. The distribution of x_j should cover a greater range from a distribution of a single X_i than x_1, \dots, x_N. <p>2. $\mu(x)$ function evaluations $\mu(x_j)$</p> <p>For all $j = 1, \dots, N$, we compute $\mu(x_j)$ either using a library or a user writing computer code.</p> <p>3. Approximation of $\mu(x) \in \tilde{\mu}$</p> <ul style="list-style-type: none"> Weights $w_j(x)$ depending on parameters x for reweighting the sample x_1, \dots, x_N according to the distribution of X_i. $w_j(x) = \frac{f(x_j)}{N \cdot f(x)}$ where f_j and f_x are strictly positive densities. Approximation of $\mu(x) \in \tilde{\mu}$ for different random variables X_i without additional function evaluations of μ: $\mu(x) \approx \sum_{j=1, \dots, N} w_j(x) \mu(x_j)$ <p>4. Approximation of $\underline{P}(\mu \leq 0)$ and $\overline{P}(\mu \leq 0)$</p> <p>For the computation of the upper/lower probabilities $\underline{P}(\mu \leq 0)$ and $\overline{P}(\mu \leq 0)$ we:</p> <ul style="list-style-type: none"> use a grid of representative parameter values x_j, estimate the probabilities $P(\mu(x_j) \leq 0)$ at the grid points x_j by means of MC simulation, and take the maximum/minimum value: $\underline{P}(\mu \leq 0) = \min_{j=1, \dots, N} P(\mu(x_j) \leq 0)$ $\overline{P}(\mu \leq 0) = \max_{j=1, \dots, N} P(\mu(x_j) \leq 0)$ <p>Effort: N_{MC} Monte Carlo samplings, N_{MC} function evaluations of μ.</p>	<p>Simulation of a random set</p> <p>Goal: Approximation of $\mu(x) \in \tilde{\mu}$ by means of Monte Carlo simulation.</p> <p>1. Generation of a random set through μ</p> <ul style="list-style-type: none"> $\tilde{\mu} = \bigcup_{j=1, \dots, N} \{x_j\}$ $\tilde{\mu} = \bigcup_{j=1, \dots, N} \{x_j\}$ $\tilde{\mu} = \bigcup_{j=1, \dots, N} \{x_j\}$ <p>2. Cumulative distribution functions</p> <ul style="list-style-type: none"> $F_j(x) = P(\mu(x_j) \leq x)$ $F_j(x) = P(\mu(x_j) \leq x)$ $F_j(x) = P(\mu(x_j) \leq x)$ <p>3. Algorithms for computing $\tilde{\mu}$</p> <ul style="list-style-type: none"> Generate x_1, \dots, x_N distributed as X_i. For each x_j, estimate $\mu(x_j) = \mu(x_j)$ using grid points x_j. Effort: N_{MC} Monte Carlo samplings of μ. <p>4. Cost saving methods</p> <p>Approximation of $\mu(x) \in \tilde{\mu}$ by a surrogate model $\tilde{\mu}$.</p> <p>Surrogate model $\tilde{\mu}$: Storing point Collocation points x_j, $j = 1, \dots, N_{\text{MC}}$ in \mathbb{S}^n and $\mu(x_j)$ function evaluations $\mu(x_j) \in \mathbb{R}$.</p> <p>The levels are at hand: $\tilde{\mu} = \bigcup_{j=1, \dots, N_{\text{MC}}} \{x_j\}$.</p> <p>1. Surrogate model $\tilde{\mu}$ of the map $\mu: \mathbb{S}^n \rightarrow \mathbb{R}$</p> <p>To obtain the lower bound $\underline{P}(\mu \leq 0)$ in the above algorithm we replace μ by $\tilde{\mu}$ through points x_j:</p> <p>$\underline{P}(\mu \leq 0) = \min_{j=1, \dots, N_{\text{MC}}} P(\mu(x_j) \leq 0)$</p> <p>Effort: 1 surrogate model $\tilde{\mu}$, N_{MC} evaluations of μ and N_{MC} evaluations of μ.</p> <p>2. Surrogate model $\tilde{\mu}$ of maps $\Omega \rightarrow \mathbb{R}^m$</p> <p>Collocation points x_j are put back to Ω.</p> <p>For each x_j and x_j, we get a collocation point $\omega_j = X_{i, \omega_j}$ in Ω.</p> <p>Clearly: $\mu(x_j) = \mu(x_j)$ for every x_j.</p> <p>Effort: N_{MC} surrogate models $\tilde{\mu}$, N_{MC} evaluations of μ, $i = 1, \dots, N_{\text{MC}}$, and N_{MC} evaluations of μ.</p>
<p>Effort: N_{MC} Monte Carlo samplings, N_{MC} function evaluations of μ.</p>	<p>with standard normally distributed sample $x_j = 0$, $N_{\text{MC}} = 100000$.</p> <p>Evaluations of $\mu: N_{\text{MC}} = 100000$ (11.4) = 6600000.</p>  <p>Simulation of a family of random variables</p> <ul style="list-style-type: none"> Failure probability $P(X_i \leq 0)$ of the beam for a fixed pair $(\mu, \omega) \in A$: with N_{MC} Monte Carlo samplings $\mu(x_j) \in \mathbb{R}$ and weights $w_j(x) = \frac{f(x_j)}{N_{\text{MC}} \cdot f(x)}$ Basic sample x_1, \dots, x_N (100000) distributed as $X_i = N(0, 1)$. $\overline{P}(\mu \leq 0) = \sup_{j=1, \dots, N_{\text{MC}}} P(\mu(x_j) \leq 0) \approx 0.221$ using grid points $(\mu, \omega) = (-20, 21, \dots, 30)$ and $\omega_j = 0.5, 1.5, \dots, 3$. Evaluations of $\mu: N_{\text{MC}} = 100000$.  <p>5. Advantage of surrogate models $\tilde{\mu}$ on Ω</p> <p>One may use orthogonal polynomials with respect to the measure μ in the Gaussian case it means Hermite expansion.</p>