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 \( X \) generated by \( \{g(X_\lambda)\}_{\lambda \in \Lambda} \).
## Two approaches

### 1 Family \( \{X_\lambda\}_{\lambda \in \Lambda} \) of random variables
- Probability space \((\Omega, \Sigma, m)\).
- 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 \( X_\lambda \):
  \[ P(X_\lambda \in B) = \int_{\Omega} \mathbb{1}_{X_\lambda(\omega) \in B} \, dm(\omega). \]
  (for initial analysis we drop the map \( g \))

### 2 Random set \( \mathcal{X} \) based on \( \{X_\lambda\}_{\lambda \in \Lambda} \)
- Set-valued map \( \mathcal{X} : \Omega \to \mathbb{R} \) defined by
  \[ \mathcal{X}(\omega) = \{X_\lambda(\omega) : \lambda \in \Lambda\}. \]
- \( \mathcal{X} \) is a random set, if upper/lower inverses
  \[ \mathcal{X}^-(B) = \{\omega \in \Omega : X(\omega) \cap B \neq \emptyset\}, \]
  \[ \mathcal{X}^-(B) = \{\omega \in \Omega : X(\omega) \subseteq B\} \]
  are measurable subsets of \( \Omega \).
## Two approaches

1. **Family \( \{X_\lambda\}_{\lambda \in \Lambda} \) of random variables**
   - Probability space \((\Omega, \Sigma, m)\).
   - 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 \( X_\lambda \):
     \[ P(X_\lambda \in B) = \int_\Omega 1_{X_\lambda(\omega) \in B} \, dm(\omega). \]
     (for initial analysis we drop the map \( g \))

### Lower/upper probabilities for \( \{X_\lambda\}_{\lambda \in \Lambda} \)

\[
\underline{P}(B) = \inf_{\lambda \in \Lambda} P(X_\lambda \in B) = \inf_{\lambda \in \Lambda} \int_\Omega 1_{X_\lambda(\omega) \in B} \, dm(\omega)
\]
\[
\overline{P}(B) = \sup_{\lambda \in \Lambda} P(X_\lambda \in B) = \sup_{\lambda \in \Lambda} \int_\Omega 1_{X_\lambda(\omega) \in B} \, dm(\omega)
\]

2. **Random set \( X \) based on \( \{X_\lambda\}_{\lambda \in \Lambda} \)**
   - Set-valued map \( X : \Omega \to \mathbb{R} \) defined by
     \[ X(\omega) = \{X_\lambda(\omega) : \lambda \in \Lambda\}. \]
   - \( X \) is a random set, if upper/lower inverses
     \[
     \underline{X}(B) = \{\omega \in \Omega : X(\omega) \cap B \neq \emptyset\},
     \overline{X}(B) = \{\omega \in \Omega : X(\omega) \subseteq B\}
     \]
     are measurable subsets of \( \Omega \).

### Lower/upper probabilities for \( X \)

\[
\underline{P}(B) = m(\underline{X}(B)) = \int_\Omega 1_{X(\omega) \subseteq B} \, dm(\omega)
\]
\[
\overline{P}(B) = m(\overline{X}(B)) = \int_\Omega 1_{X(\omega) \cap B \neq \emptyset} \, dm(\omega)
\]
Two approaches

1. Family $\{X_\lambda\}_{\lambda \in \Lambda}$ of random variables
   - Probability space $(\Omega, \Sigma, m)$.
   - 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 $X_\lambda$:
     \[ P(X_\lambda \in B) = \int_{\Omega} 1_{X_\lambda(\omega) \in B} \, dm(\omega). \]
     (for initial analysis we drop the map $g$)

2. Random set $X$ based on $\{X_\lambda\}_{\lambda \in \Lambda}$
   - Set-valued map $X : \Omega \to \mathbb{R}$ defined by
     \[ X(\omega) = \{X_\lambda(\omega) : \lambda \in \Lambda\}. \]
   - $X$ is a random set, if upper/lower inverses
     \[ X^+(B) = \{\omega \in \Omega : X(\omega) \cap B \neq \emptyset\}, \]
     \[ X^-(B) = \{\omega \in \Omega : X(\omega) \subseteq B\} \]
     are measurable subsets of $\Omega$.

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

<table>
<thead>
<tr>
<th>Lower/upper probabilities for ${X_\lambda}_{\lambda \in \Lambda}$</th>
<th>Lower/upper probabilities for $X$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\underline{P}(B) = \inf_{\lambda \in \Lambda} P(X_\lambda \in B) = \inf_{\lambda \in \Lambda} \int_{\Omega} 1_{X_\lambda(\omega) \in B} , dm(\omega)$</td>
<td>$\underline{\tilde{P}}(B) = m(X^+(B)) = \int_{\Omega} 1_{X(\omega) \subseteq B} , dm(\omega)$</td>
</tr>
<tr>
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</table>

**Theorem**

\[ \underline{\tilde{P}} \leq \underline{P} \leq \overline{P} \leq \overline{\tilde{P}} \]

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

- **Probability space:** \((\Omega, \Sigma, m) = (\mathbb{R}, \mathcal{B}(\mathbb{R}), m), \quad m(B) = \int_{\mathbb{R}} 1_{\omega \in B} \frac{1}{\sqrt{2\pi}} e^{-\omega^2/2} \, d\omega.\)

- **Family** \(\{X_{(\mu, \sigma)}\}_{(\mu, \sigma) \in \Lambda} : X_{(\mu, \sigma)}(\omega) = \sigma \omega + \mu \implies X_{(\mu, \sigma)} \sim \mathcal{N}(\mu, \sigma^2).\)

- \(\Lambda = [\mu, \bar{\mu}] \times [\sigma, \bar{\sigma}] = [-0.5, 2] \times [1, 2], \quad B = [1, 2.5].\)

\[
\begin{align*}
X(\omega) &= \{X_{\lambda}(\omega) : \lambda \in \Lambda\} = [\underline{X}(\omega), \overline{X}(\omega)] \\
\underline{X}(\omega) &= \inf_{\mu \in [\mu, \bar{\mu}], \sigma \in [\sigma, \bar{\sigma}]} X_{(\mu, \sigma)}(\omega) = \begin{cases} 
\sigma \omega + \mu & \omega < 0 \\
\sigma \omega + \bar{\mu} & \omega \geq 0
\end{cases} \\
\overline{X}(\omega) &= \sup_{\mu \in [\mu, \bar{\mu}], \sigma \in [\sigma, \bar{\sigma}]} X_{(\mu, \sigma)}(\omega) = \begin{cases} 
\sigma \omega + \mu & \omega < 0 \\
\bar{\sigma} \omega + \mu & \omega \geq 0
\end{cases}
\end{align*}
\]

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

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

- \(\underline{P}(B) = m(\underline{X}^{-}(B)) = m(\emptyset) = 0.0000\)

- \(\overline{P}(B) = m(\overline{X}^{-}(B)) = m([-1, 3]) = \Phi(3) - \Phi(-1) = 0.8400\)
Simulation of a family \( \{X_\lambda\}_{\lambda \in \Lambda} \) of random variables

### 1 Basic sample \( x_1, \ldots, x_{N_{\text{samp}}} \)

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

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

- 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 \( \lambda \) is computed by **reweighting** the original sample.
- Weights \( w_k(\lambda) \) depending on parameters \( \lambda \) for reweighting the sample \( x_1, \ldots, x_{N_{\text{samp}}} \) according to the distribution of \( X_\lambda \):
  \[
  w_k(\lambda) = \frac{f_{X_\lambda}(x_k)}{f_{X_*}(x_k)} \cdot \frac{1}{N_{\text{samp}}} = \frac{f_{\text{new}}(x_k)}{f_{\text{old}}(x_k)} \cdot \frac{1}{N_{\text{samp}}}
  \]
  where \( f_{X_\lambda} \) and \( f_{X_*} \) are strictly positive densities.
- \( P(g(X_\lambda) \leq y) \) for different \( X_\lambda \) **without additional function evaluations** of \( g \):
  \[
  P(g(X_\lambda) \leq y) \approx \sum_{k=1}^{N_{\text{samp}}} \mathbb{1}_{g(x_k) \leq y} \cdot w_k(\lambda) = \sum_{k=1}^{N_{\text{samp}}} \mathbb{1}_{g(x_k) \leq y} \cdot w_k(\lambda).
  \]
Simulation of a family $\{X_\lambda\}_{\lambda \in \Lambda}$ of random variables

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

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

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

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

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

**Effort:** $N_{\text{grid}} \cdot N_{\text{samp}}$ reweightings, $N_{\text{samp}}$ expensive function evaluations of $g$. 
Simulation of a random set $X$

1. Propagation of a random set through $g$

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

2. Cumulative distribution functions

- $\overline{F}(y) = \tilde{P}(g \leq y)$, $\underline{F}(y) = \bar{P}(g \leq y)$
- $\overline{F}(y) = P((\infty, y] \cap [\underline{g}, \overline{g}] \neq \emptyset) = P(\underline{g} \leq y) = \underline{F}(y)$
- $\underline{F}(y) = P([\underline{g}, \overline{g}] \subset (-\infty, y]) = P(\overline{g} \leq y) = \overline{F}(y)$

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

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

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

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Simulation of a random set $X$

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

Starting point: Collocation points $x_j, j = 1, \ldots, N_{coll}$, 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 $\tilde{g}$: $\underline{g}(\omega_n) \approx \min_{i=1,\ldots,N_{grid}} \tilde{g}(X_\lambda_i(\omega_n))$.

Effort: One surrogate model $\tilde{g}$,

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

B Surrogate models $\tilde{g}_i$ of maps $\Omega \rightarrow g \circ X_\lambda$:

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

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 $\Omega$:

- Use of orthogonal polynomials with respect to the measure $m$.
- In the Gaussian case it means Hermite expansion.
Imprecise random variables, random sets, and Monte Carlo simulation

Given:
Simulate a family of random variables

Family:
- Probability space $(\Omega, \mathcal{F}, \mathbb{P})$ of random variables
- $X_1, X_2, \ldots, X_n$ are measures of the sample
- $g(\cdot)$ is a continuous function
- $g(x_1, x_2, \ldots, x_n)$ is a real-valued function

Weight function evaluations:
For all $i = 1, \ldots, N_{\text{eval}}$ we compute $g(x_i)$ using $g(x_i)$ directly or a cost-saving surrogate model $g^\#$.

Simulation of a family of random variables
Goal: Approximation of $P(g(X_1) \leq t), P(g(X_2) \leq t)$ by means of Monte Carlo simulation using only one sample for all random variables $X_1, X_2, \ldots, X_n$.

Basic sample evaluation:
1. We generate a sample $x_1, \ldots, x_n$ which distributed as a random variable $X_i$.
2. The distribution of $X_i$ should cover a greater range than a distribution of a single $x_i$.

Approximation of $P(g(X_i) \leq t)$:
1. Probability $P(g(X_i) \leq t)$ for fixed $X_i$ is computed by reweighting the original sample.
2. Weights $w_i(x_i)$, depending on parameters, for reweighting the sample $x_1, \ldots, x_n$ according to the distribution of $X_i$.

Cumulative distribution functions:
- $P(g(X_i) \leq t)$ is approximated using grid points $x_i$.

Algorithm for computing $P(g(X_i) \leq t)$:
- Generate $n_i$ samples $x_i$ distributed as $X_i$.
- For each $x_i$, compute $g(x_i)$ using a grid point $x_i$.
- Effect: $n_i$ evaluations $g(x_i)$. 

Cost-saving methods:
Approximation of $P(g(X_i) \leq t)$ using a surrogate model $g^\#$.

Surrogate model $g^\#$ at a grid point $x_i$:
- Collocation points $x_i^{\text{col}}$ and $x_i^{\text{test}}$ are used to evaluate $g(x_i)$ at the grid point $x_i$.

Example:
- Beam tested on spring with uncertain spring constant

Simulation of a random set:
- Gold points $(x_i, y_i)$ with $x_i \in [0, 20], y_i \in [-5, 5]$
- Focal set $M$ of the random set $\alpha$ is approximated by $\hat{M} = \{ x | x \in M \}$
- Approximation of the upper probability of failure of the beam by means of Monte Carlo simulation:

Simulation of a family of random variables:
- Full range probability $P(X_i \in B)$ of the beam for fixed $(x_i, y_i)$ is approximated by $\hat{P}(X_i \in B)$ using grid points $(x_i, y_i)$.

Basic sample $x_1, \ldots, x_{N_{\text{sam}}}$, $\hat{P}(X_i \in B) = 10^{-6}$.

Upper probability of failure is approximated by $\hat{P}(\hat{X}_i \in \hat{B}) = \frac{1}{N_{\text{sam}}} \sum_{j=1}^{N_{\text{sam}}} P(x_j \in \hat{B})$.

Example:
- Given: Limit state function $y$ and $(\tilde{x}_j)_{j=1}^{N_{\text{sam}}}$ for spring constant $c_j$ as in the above example, but here with $\tilde{x}_j \in \mathcal{N}(\mu_j, \sigma_j)$, $\sigma_j = 0.3x_j$.
- Goal: Upper/lower probabilities of failure.

Please visit our poster for more details and numerical examples!

Thank you for your attention!

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10 / 10