Multifidelity Global Sensitivity Analysis

Elizabeth Qian
April 4, 2023
MASCOT-NUM 2023 | Le Croisic

Financial support from the following programs is gratefully acknowledged: the National Science Foundation Graduate Research Fellowship Program; the Fannie and John Hertz Foundation; the Air Force Center of Excellence on Multi-Fidelity Modeling of Rocket Combustor Dynamics, Award Number FA9550-17-1-0195; the US Department of Energy, Office of Advanced Scientific Computing Research (ASCR), Applied Mathematics Program, awards DE-FG02-08ER2585 and DE-SC0009297, as part of the DiaMonD Multifaceted Mathematics Integrated Capability Center; and the National Aeronautics and Space Administration (NASA) under Award No. 80GSFC21M0002.
The need for uncertainty quantification

Engineering/scientific systems subject to many uncertainties
- Unknown parameters
- Uncertain operating conditions
- Variation in manufacturing process

These uncertainties can have high-consequence impacts:
- Cost
- Risk of system failure
- (In)efficiency
Probabilistic uncertainty propagation

Engineering/scientific systems subject to many uncertainties
  • uncertain inputs/parameters can be modeled as random variables

Random inputs lead to random variation in QI

Simulation $f$

$Y = f(Z_1, Z_2, ...)$
Sensitivity analysis

How sensitive is the QI to changes in each input?
- If QI is not sensitive to some inputs, can limit design/decision space
- If QI very sensitive to some inputs, can invest more effort in reducing associated uncertainty

Derivatives of QI w.r.t. inputs are a local measure of sensitivity
- They tell us how much QI will change if the inputs are varied from a single point
- can exhibit significant variation over the range of possible input values
Outline

1. Sobol’ global sensitivity analysis
   - Theory
   - Computation

2. Multifidelity Monte Carlo methods

3. Numerical results
Variance-based global sensitivity analysis

Random inputs or parameters $Z_1$, $Z_2$, $Z_3$

Simulation $f$

Quantity of Interest (QoI) $Y = f(Z_1, Z_2, ...)$

Variance-based sensitivity analysis
- Quantifies how much each random input contributes to variation in QoI

$\text{Var}[Y]$
Variance-based global sensitivity analysis: Theoretical foundation

Input/output domains:
\[ Z \in \mathbb{R}^d, \ Y \in \mathbb{R} \]

Model:
\[ f : Z \to Y \]

Input random variable:
\[ Z : \Omega \to Z \]
- measure \( \mu \)
- independent components
- Probability tuple: \( (\Omega, \mathcal{F}, \mathbb{P}) \)

If \( f \) is square-integrable w.r.t. \( \mu \), then:
- \( \mathbb{E}[f(Z)], \ \text{Var}[f(Z)] < \infty \), and
- \( f \) can be written as the sum of functions of subsets of its inputs:
\[
 f(z) = f_0 + \sum_{i=1}^{d} f_i(z_i) + \sum_{i,j=1}^{d} f_{ij}(z_i, z_j) + \cdots + f_{1\ldots d}(z_1, \ldots, z_d)
\]

This is the ANOVA HDMR (analysis-of-variance high-dimensional model representation).
Variance-based global sensitivity analysis: Theoretical foundation

ANOVA HDMR:

\[ f(z) = f_0 + \sum_{i=1}^{d} f_i(z_i) + \sum_{i,j=1}^{d} f_{ij}(z_i, z_j) + \cdots + f_{1\ldots d}(z_1, \ldots, z_d) \]

Variance can be similarly decomposed:

\[ \text{Var}[f(Z)] = \sum_{i=1}^{d} \text{Var}[f_i(Z_i)] + \sum_{i,j=1}^{d} \text{Var}[f_{ij}(z_i, z_j)] + \cdots + \text{Var}[f_{1\ldots d}(Z_1, \ldots, Z_d)] \]

Sobol’ sensitivity indices:

\[ s_i = \frac{\text{Var}[f_i(Z_i)]}{\text{Var}[f(Z)]} \]

Sobol’ main index

\[ s'_i = \frac{\text{Var}[\text{all } f_* \text{ where } i \text{ is in } *]}{\text{Var}[f(Z)]} \]

Sobol’ total index
Sobol’ sensitivity analysis

Simulation $f$

Quantity of Interest (QoI) $Y = f(Z_1, Z_2, ...)$

Random inputs or parameters

**Sobol’ main index:** $s_i \in [0,1]$
- how much of the $\text{Var}[Y]$ pie is due to $Z_i$ alone

**Sobol’ total index:** $s_i' \in [0,1]$
- how much of $\text{Var}[Y]$ pie does $Z_i$ contribute to in any way (includes interactions with other inputs)
Computing Sobol’ indices

Sobol’ indices can be expressed using conditional expectations:

$$s_i = \frac{\text{Var}[f_i(Z_i)]}{\text{Var}[f(Z)]} = \frac{\text{Var}[\mathbb{E}[Y|Z_i]]}{\text{Var}[f(Z)]}$$

$$s_i' = \frac{\text{Var}[\text{all } f_* \text{ where } i \text{ is in } *]}{\text{Var}[f(Z)]} = 1 - \frac{\text{Var}[\mathbb{E}[Y|Z_{\sim i}]]}{\text{Var}[f(Z)]}$$

We compute Sobol’ indices by estimating these conditional expectations via **Monte Carlo methods**
Sobol’ main indices: naïve estimation

\[ S_j = \frac{\text{Var}(\mathbb{E}[Y|Z_j])}{\text{Var}(Y)} \]

\[ \hat{s}_j = \frac{\hat{V}_j}{\hat{V}} \]

Naïve approach:

for \( j = 1: d \)

sample \( \{z_j^{\{i\}}\}_{i=1}^n \)

for \( i = 1: n \)

sample \( \{(z_1, \ldots, z_{j-1}, z_{j+1}, \ldots, z_d)^{(k)}\}_{k=1}^n \)

\[ y_{ik} = f(z_1, \ldots, z_{j-1}, z_j, z_{j+1}, \ldots, z_d) \]

\[ \hat{y}_i = \text{mean}(y_{i1}, y_{i2}, \ldots, y_{in}) \]

\[ \hat{V}_j = \text{var}(\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_n) \]
Sobol’ main indices: ‘pick-freeze’ estimation

Naïve approach:

for $j = 1: d$

sample $\{z_j^{(i)}\}_{i=1}^n$

for $i = 1: n$

sample $\{(z_1, \ldots, z_{j-1}, z_j, z_{j+1}, \ldots, z_d)^{(k)}\}_{k=1}^n$

for $k = 1: n$

$y_{jik} = f(z_1, \ldots, z_{j-1}, z_j, z_{j+1}, \ldots, z_d)$

$\hat{y}_{ji} = \text{mean}(y_{ji1}, y_{ji2}, \ldots, y_{jin})$

$\hat{V}_j = \text{var}(\hat{y}_{j1}, \hat{y}_{j2}, \ldots, \hat{y}_{jn})$

Pick-freeze approach*:

sample $\{(z_1, \ldots, z_d)^{(i)}\}_{i=1}^n$

for $j = 1: d$

for $i = 1: n$

$y_{ji} = f(z_1, \ldots, z_d)$

$\hat{V}_j = \text{mean}_i(y_{ji}y_{ji}) - \text{mean}_i(y_{ji})^2$

*see Saltelli, Janon, Owen, etc.
Estimation of Sobol’ total indices

Naïve approach:
for $j = 1: d$

sample $\{(z_1, \ldots, z_{j-1}, z_{j+1}, \ldots, z_d)^{(i)}\}_{i=1}^{n}$

for $i = 1: n$

sample $\{Z_j^{(k)}\}_{k=1}^{n}$

for $k = 1: n$

$y_{jik} = f(z_1, \ldots, z_{j-1}, z_j, z_{j+1}, \ldots, z_d)$

$\hat{y}_{ji} = \text{mean}(y_{ji1}, y_{ji2}, \ldots, y_{jin})$

$\hat{V}_j = \hat{V} - \text{var}(\hat{y}_{j1}, \hat{y}_{j2}, \ldots, \hat{y}_{jn})$

$s'_i = 1 - \frac{\text{Var}[\mathbb{E}[Y|Z_{\sim i}]]}{\text{Var}[f(Z)]}$

$\hat{s}'_j = \frac{\hat{V}'_j}{\hat{V}}$
Estimation of Sobol’ total indices

Naïve approach:
for \( j = 1: d \)
    sample \( \{(z_1, \ldots, z_{j-1}, z_j, z_{j+1}, \ldots, z_d)^{(i)}\}_{i=1}^{n} \)
for \( i = 1: n \)
    sample \( \{z_j^{(k)}\}_{k=1}^{n} \)
    for \( k = 1: n \)
        \( y_{jik} = f(z_1, \ldots, z_{j-1}, z_j, z_{j+1}, \ldots, z_d) \)
        \( \hat{y}_{ji} = \text{mean}(y_{ji1}, y_{ji2}, \ldots, y_{jin}) \)
    \( \hat{V}'_j = \hat{V} - \text{var}(\hat{y}_{j1}, \hat{y}_{j2}, \ldots, \hat{y}_{jn}) \)

Pick-freeze approach*:
for \( j = 1: d \)
    sample \( \{(z_1, \ldots, z_d)^{(i)}\}_{i=1}^{n} \)
    for \( i = 1: n \)
        \( y_{ji} = f(z_1, \ldots, z_d) \)
        \( \hat{V}_j = \text{mean}_i(y_{ji}, y_{ji}) - \text{mean}_i(y_{ji})^2 \)
        \( \hat{V}'_j = \hat{V} - \text{mean}_i(y_{ji}y_{ji}) - \text{mean}_i(y_{ji})^2 \)
Sobol estimation is expensive and cumbersome

Naïve approach:

\[
\text{for } j = 1: d
\]
\[
\text{sample } \{z_{j (i)}\}^n_{i=1}
\]
\[
\text{requires } n^2 \text{ evaluations of } f \text{ per index}
\]
\[
n^2 d \text{ evals for all } d \text{ main indices}
\]
\[
y_{ijk} = f(z_1, \ldots, z_{j-1}, z_j, z_{j+1}, \ldots, z_d)
\]
\[
y_{ji} = \text{mean}(y_{ji1}, y_{ji2}, \ldots, y_{jin})
\]
\[
\hat{y}_j = \text{var}(\hat{y}_{j1}, \hat{y}_{j2}, \ldots, \hat{y}_{jn})
\]

Pick-freeze approach*:

\[
\text{sample } \{(z_1, \ldots, z_d)^{(i)}\}^n_{i=1}
\]
\[
\text{requires } n(d + 1) \text{ evaluations of } f \text{ for all } d \text{ main and } d \text{ total indices}
\]
\[
y_{ji} = f(z_1, \ldots, z_d)
\]
\[
\hat{y}_{ji} = \text{mean}(y_{ji1}, y_{ji2}, \ldots, y_{jin})
\]
\[
\hat{y} = \text{mean}_i(\hat{y}_{ji} - \text{mean}_i(\hat{y}_{ji}))^2
\]

*see Saltelli, Janon, Owen, etc.
Sobol’ main indices:
Rank statistics estimation

Pick-freeze approach:

\[
sample \{ (z_1, ..., z_d)^{(i)} \}_{i=1}^n
\]
\[
sample \{ (z_1, ..., z_d)^{(i)} \}_{i=1}^n
\]
\[
for j = 1: d
\]
\[
for i = 1: n
\]
\[
y_{ji} = f(z_1, ..., z_d)
\]
\[
y_{ji} = f(z_1, ..., z_{j-1}, z_j, z_{j+1}, ..., z_d)
\]
\[
\hat{V}_j = \text{mean}_i (y_{ji}y_{ji}) - \text{mean}_i (y_{ji})^2
\]

Rank statistics approach*:

\[
sample \{ (z_1, ..., z_d)^{(i)} \}_{i=1}^n
\]
\[
for i = 1: n
\]
\[
y_i = f(z_1, ..., z_d)
\]
\[
for j = 1: d
\]
\[
\hat{V}_j = \text{mean}_i (y_i y_{R_j(i)}) - \text{mean}_i (y_i)^2
\]

\[v_j = \text{mean}_i (y_{R_j(i)}) - \text{mean}_i (y_i)^2\]

where \(y_{R_j(i)}\) is the \(y\)-value that comes after \(y_i\) when the \(y\)'s are ordered by increasing \(z_j\)

*Gamboa, Gremaud, Klein, & Lagnoux 2021
Rank statistics estimators do not require special experimental design

Pick-freeze approach:

\[ \text{sample } \{ (z_1, \ldots, z_d)^{(i)} \}_{i=1}^n \]
\[ \text{sample } \{ (z_1, \ldots, z_d)^{(i)} \}_{i=1}^n \]

requires \( n(d + 1) \) evaluations of \( f \)
for all \( d \) main and \( d \) total indices

\[ y_{ji} = f(z_1, \ldots, z_d) \]
\[ y_{ji} = f(z_1, \ldots, z_d) \]

and the ability to evaluate \( f \) at
pick-freeze inputs

\[ \hat{\nu}_j = \text{mean}_i(y_{ji}y_{ji}) - \text{mean}_i(y_{ji})^2 \]

Rank statistics approach*:

\[ \text{sample } \{ (z_1, \ldots, z_d)^{(i)} \}_{i=1}^n \]
\[ \text{for } i = 1: n \]
\[ y_i = f(z_1, \ldots, z_d) \]
\[ \text{for } j = 1: d \]

requires \( n \) evaluations of \( f \)
at arbitrary i.i.d. inputs

\[ \hat{\nu}_j = \text{mean}_i(y_{iR_j(i)}) - \text{mean}_i(y_i)^2 \]

where \( y_{iR_j(i)} \) is the \( y \)-value that comes after
\( y_i \) when the \( y \)'s are ordered by increasing \( z_j \)

*Gamboa et al 2021
Summary: Sobol’ sensitivity analysis

Variance of a model $f$ can be decomposed into portions attributable to each input and each subset of inputs.

Sobol’ indices give the % of model variance attributable to that input alone (main index) or any of its interactions (total index).

Sobol’ indices can be estimated using Monte Carlo methods.

- Many estimators in the literature: authors include Borgonovo, Iooss, Janon, Kucherenko, Li, Mahadevan, Mauntz, Owen, Saltelli, Sobol’, and more.
Outline

1. Sobol’ global sensitivity analysis

2. Multifidelity Monte Carlo methods
   - Variance reduction using control variates
   - Model management strategy

3. Numerical results
Motivating application: Space mission design

Space mission design is
  • Multidisciplinary
  • Subject to many uncertainties
  • Costly (time, money, and effort)

Case study:
  • QI: optical wavefront error in James Webb Space Telescope
  • Uncertain inputs are material properties for different telescope substructures
Sobol’ index estimation for JWST

• 66 uncertain material properties

• Model: thermal simulation of JWST as it turns to/away from the sun
  • Multiple coupled commercial software
  • Computational budget severely resource-limited in terms of time + nodes + licenses

• 2 months of real-world time to obtain enough samples for pick-freeze estimation of just 5 Sobol’ indices

...need more efficient methods to enable Sobol’ analysis for applications of this scale.
Variance reduction using control variates

Consider Monte Carlo estimation of the mean:

$$\hat{\mu}_N^Y = \frac{1}{N} \sum_{i=1}^{N} y_i = \frac{1}{N} \sum_{i=1}^{N} f(z_i)$$

$$\text{Var}[\hat{\mu}_N^Y] = \frac{\text{Var}[Y]}{N}$$

Let $W = g(Z)$. Then we define the following estimator:

$$\hat{\mu}_Y^{c.v.} = \hat{\mu}_Y^n + \alpha(\hat{\mu}_W^n - \mu_W)$$

$$\mathbb{E}[\hat{\mu}_Y^{c.v.}] = \mathbb{E}[\hat{\mu}_Y^n] + \alpha(\mathbb{E}[\hat{\mu}_W^n] - \mu_W) = \mu_Y$$

$$\text{Var}[\hat{\mu}_Y^{c.v.}] = \text{Var}[\hat{\mu}_Y^n] + \alpha^2\text{Var}[\hat{\mu}_W^n] + 2\alpha\text{Cov}[\hat{\mu}_Y^n, \hat{\mu}_W^n]$$
Variance reduction using control variates

\[ \hat{\mu}_Y^{c.v.} = \hat{\mu}_Y^n + \alpha (\hat{\mu}_W^n - \mu_W) \]

\[ \mathbb{E} [\hat{\mu}_Y^{c.v.}] = \mathbb{E} [\hat{\mu}_Y^n] + \alpha (\mathbb{E} [\hat{\mu}_W^n] - \mu_W) = \mu_Y \]

\[ \text{Var}[\hat{\mu}_Y^{c.v.}] = \text{Var}[\hat{\mu}_Y^n] + \alpha^2 \text{Var}[\hat{\mu}_W^n] + 2\alpha \text{Cov}[\hat{\mu}_Y^n, \hat{\mu}_W^n] \]

Optimal \( \alpha = -\frac{\text{Cov}[\hat{\mu}_Y^n, \hat{\mu}_W^n]}{\text{Var}[\hat{\mu}_W^n]} = \frac{\rho \sigma_Y}{\sigma_W} \) yields

\[ \text{Var}[\hat{\mu}_Y^{c.v.}] = (1 - \rho^2) \text{Var}[\hat{\mu}_Y^n] \]

Estimator has lower variance if high correlation between \( W \) and \( Y \)
Multifidelity Monte Carlo uses low-fidelity engineering models as control variates

Recall $Y = f(Z)$ and $W = g(Z)$.

Detailed analysis of MFMC mean estimator in [1] yields

- Model selection criteria to achieve variance reduction
- Optimal sample allocation strategy (among diff models) for fixed budget

$f$ is expensive high-fidelity model
- e.g. discretized PDE on fine mesh

$g$ is cheaper lower-fidelity model
- Discretized PDE on coarse mesh
- Projection-based reduced model
- Simplified physics model
- Data-fit model

Multifidelity variance and Sobol estimators introduced in [2]

Multifidelity estimation of variance and Sobol’ indices

Q. et al SIAM JUQ 2018
• Apply control variate approach to variance and pick-freeze Sobol’ numerator estimators
• Can lead to negative variance/Sobol’ index estimates
• Analysis of MSE of multifidelity variance estimator

Cataldo, Q., & Auclair 2022:
• Multifidelity rank statistics estimators
• Case study on James Webb Space Telescope

Maurais, Alsup, Peherstorfer, & Marzouk 2023
• Multifidelity covariance estimation in the log-Euclidean geometry (enforces positivity)
Summary: Multifidelity Monte Carlo

Multifidelity methods combine high- and low-fidelity model evaluations:

- **Low-fidelity** model samples reduce estimator variance
- **High-fidelity** model samples guarantee estimator unbiasedness

Contrast with:

- High-fidelity only: unbiased, but slow
- Low-fidelity only: fast, but biased

Compare with **multilevel** methods

- Multilevel = varying grid resolution
- Multifidelity: includes larger variety of low-fidelity model types
Outline

1. Sobol’ global sensitivity analysis
2. Multifidelity Monte Carlo methods
3. Numerical results
   • Convection-diffusion-reaction example
   • JWST wavefront error sensitivity
Example: 2D Convection-Diffusion-Reaction

\[ \frac{\partial x}{\partial t} = \Delta x - U \nabla x + s(x, p) \text{ in } \Omega, \]

\[ s_i(x, p) = \nu_i \left( \frac{W_i}{\rho} \right) \left( \frac{\rho Y_F}{W_F} \right)^{\nu_F} \left( \frac{\rho Y_O}{W_O} \right)^{\nu_O} A \exp \left( -\frac{E}{RT} \right), \quad i = F, O, P, \]

\[ s_T(x, p) = s_P(x, p)Q, \]

Uncertain parameters: \( A, E, T_i, T_0, \phi \)

Monte Carlo
Multifidelity

Computational budget = 1000 minutes
2D CDR Sobol’ estimate convergence
JW Space Telescope revisited

Multifidelity pick-freeze Sobol’ estimators for JWST wavefront error with 60 day computational budget
Multifidelity rank statistics estimators

Pick-Freeze
Sobol’ main effect indices

Rank statistics

$S_m$

Variable

$S_m^c$

Variable
### Computational cost comparison

**Pick-Freeze**

**Sobol’ main effect indices**

<table>
<thead>
<tr>
<th>Method</th>
<th>Authors</th>
<th>Budget (CPU hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GSA</td>
<td>Sobol’(^5^7), Cannavò(^6^7)</td>
<td>(p = 6000)</td>
</tr>
<tr>
<td>MFGSA</td>
<td>Qian et al.(^4^7)</td>
<td>(p = 1500)</td>
</tr>
<tr>
<td>RSB GSA</td>
<td>Gamboa et al.(^7^2)</td>
<td>(p = 188)</td>
</tr>
<tr>
<td>RSB MFGSA</td>
<td>Cataldo et al.—this paper</td>
<td>(p = 47)</td>
</tr>
</tbody>
</table>

**Rank statistics**

### Chart Details

- **HF** (\(m = 80\))
- **MR** (\(n = 28, 65, 99, 209110\))
Summary: Numerics

Multifidelity control variates reduce estimator variance for Sobol’ sensitivity analysis for both model problems and at-scale application.

Multifidelity strategy yields “best of both worlds” – accuracy of high-fidelity with speed of low-fidelity.

Multifidelity global sensitivity analysis enables identification of most important inputs at reduced cost.
Summary: Overall

Sobol index estimation quantifies the relative influence of different uncertain inputs on an uncertain output.

Multifidelity pick-freeze and rank statistics estimators reduce cost, enabling Sobol index estimation in large scale applications.
Thank you

web: https://www.elizabethqian.com
email: eqian@gatech.edu

Papers:
  • Qian, Peherstorfer, O’Malley, Vesselinov, and Willcox, SIAM Journal on Uncertainty Quantification, 2018.
  • Ask/email me if you’re interested in any of the other works I’ve mentioned

Github: elizqian/mfgsa