Multifidelity Global Sensitivity Analysis

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The need for uncertainty quantification

Engineering/scientific systems subject to many uncertainties

- Unknown parameters
- Uncertain operating conditions
- Variation in manufacturing process

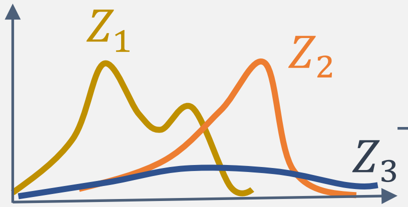
These uncertainties can have **high-consequence impacts**:

- 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
or parameters

Simulation f

Quantity of Interest (QI)

$Y = f(Z_1, Z_2, \dots)$

Random inputs lead to random variation in QI

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

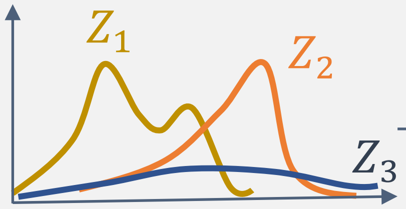
Outline

1. Sobol' global sensitivity analysis
   - Theory
   - Computation

2. Multifidelity Monte Carlo methods

3. Numerical results

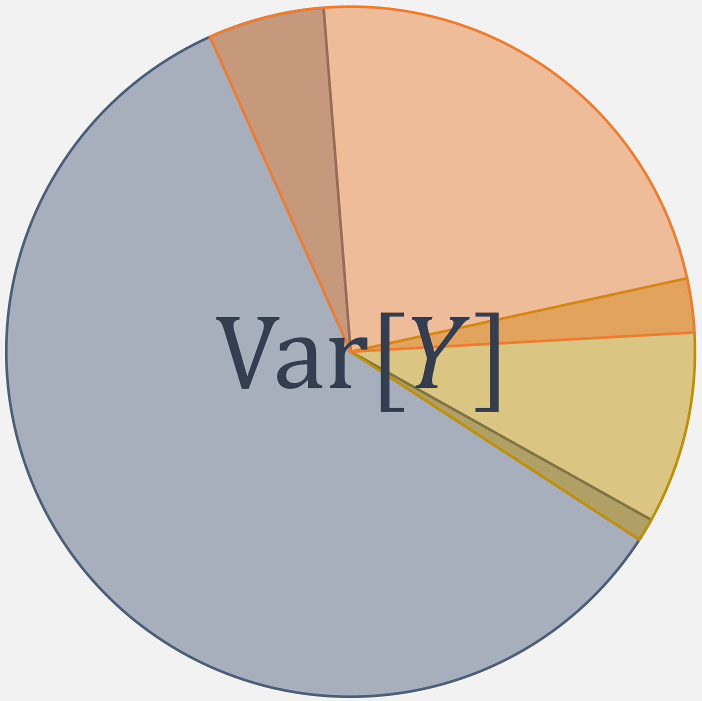
Variance-based **global** sensitivity analysis



Random inputs
or parameters

Simulation f

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



Variance-based sensitivity analysis

- Quantifies how much each random input contributes to variation in QoI

Variance-based global sensitivity analysis: Theoretical foundation

Input/output domains:

$$\mathcal{Z} \in \mathbb{R}^d, \mathcal{Y} \in \mathbb{R}$$

Model:

$$f: \mathcal{Z} \to \mathcal{Y}$$

Input random variable:

$$Z: \Omega \to \mathcal{Z}$$

- measure μ
- independent components
- Probability tuple: $(\Omega, \mathcal{F}, \mathbb{P})$

If f is square-integrable w.r.t. μ, then:

- $\mathbb{E}[f(Z)],\ \mathtt{Var}[f(Z)] < \infty$, 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:

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

Sobol' sensitivity indices:

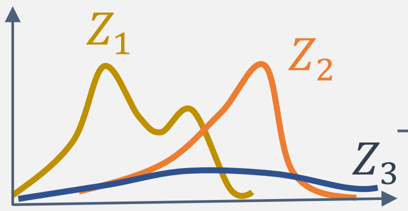
$$s_i = \frac{\mathrm{Var}[f_i(Z_i)]}{\mathrm{Var}[f(Z)]}$$

Sobol' **main** index

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

Sobol' **total** index

Sobol' sensitivity analysis



Random inputs
or parameters

Simulation f

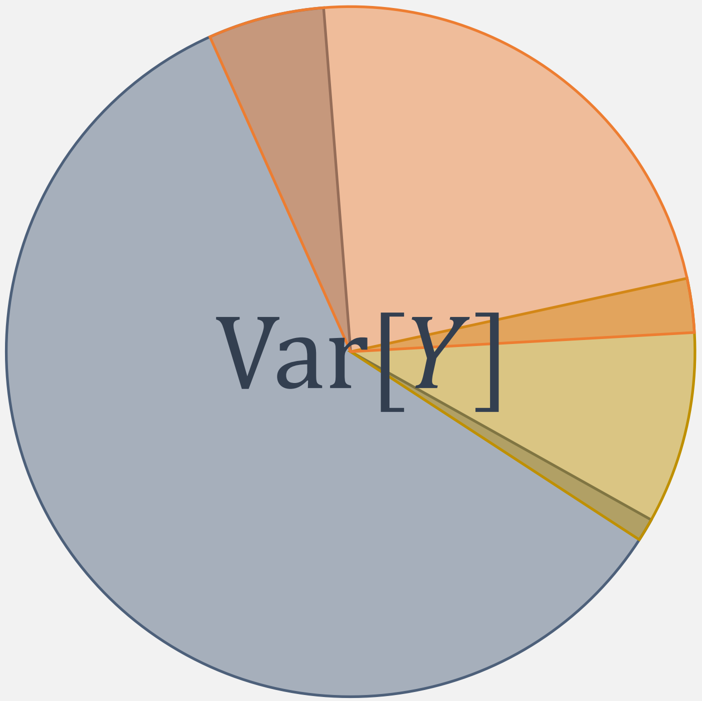
Quantity of Interest (QoI)
$Y = f(Z_1, Z_2, \ldots)$

Sobol' main index: $s_i \in [0,1]$

- how much of the $\mathrm{Var}[Y]$ pie is due to Z_i alone

Sobol' total index: $s_i' \in [0,1]$

- how much of $\mathrm{Var}[Y]$ 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:

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

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

We compute Sobol' indices by estimating these conditional expectations via **Monte Carlo methods**

Sobol' main indices: naïve estimation

$$s_j = \frac{\mathrm{Var}(\mathbb{E}[Y|Z_j])}{\mathrm{Var}(Y)}$$

$$\hat{s}_j = \frac{\hat{V}_j}{\hat{V}}$$

Naïve approach:

for $j = 1{:}d$

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

for $i = 1{:}n$

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

for $k = 1{:}n$

$y_{ik} = f\left(z_1, \dots z_{j-1}, z_j, z_{j+1}, \dots z_d\right)$

$\hat{y}_i = \mathrm{mean}(y_{i1}, y_{i2}, \dots, y_{in})$

$\hat{V}_j = \mathrm{var}(\hat{y}_1, \hat{y}_2, \dots, \hat{y}_n)$

Sobol' main indices: 'pick-freeze' estimation

Naïve approach:

for $j = 1{:}\,d$

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

  for $i = 1{:}\,n$

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

    for $k = 1{:}\,n$

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

    $\hat{y}_{ji} = \mathrm{mean}\left(y_{ji1}, y_{ji2}, \dots, y_{jin}\right)$

  $\hat{V}_j = \mathrm{var}(\hat{y}_{\mathrm{j}1}, \hat{y}_{\mathrm{j}2}, \dots, \hat{y}_{jn})$

Pick-freeze approach*:

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

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

for $j = 1{:}\,d$

  for $i = 1{:}\,n$

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

    $y_{ji} = f\left(z_1, \dots z_{j-1}, z_j, z_{j+1}, \dots z_d\right)$

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

*see Saltelli, Janon, Owen, etc.

Estimation of Sobol' total indices

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

$$\hat{s}'_j = \frac{\hat{V}'_j}{\hat{V}}$$

Naïve approach:

for $j = 1{:}d$

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

  for $i = 1{:}n$

    sample $\left\{z_j^{(k)}\right\}_{k=1}^{n}$

    for $k = 1{:}n$

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

    $\hat{y}_{ji} = \mathrm{mean}\left(y_{ji1}, y_{ji2}, \dots, y_{jin}\right)$

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

Estimation of Sobol' total indices

Naïve approach:

for $j = 1:d$

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

for $i = 1:n$

sample $\left\{z_j^{(k)}\right\}_{k=1}^{n}$

for $k = 1:n$

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

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

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

Pick-freeze approach*:

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

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

for $j = 1:d$

for $i = 1:n$

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

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

$y_{ji} = f\left(z_1, \dots z_{j-1}, z_j, z_{j+1}, \dots z_d\right)$

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

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

Sobol estimation is expensive and cumbersome

Naïve approach:

requires n^2 evaluations of f **per index**

$n^2 d$ evals for all d main indices

$n^2 d$ evals for all d total indices

Pick-freeze approach*:

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

and the ability to evaluate f at pick-freeze inputs

*see Saltelli, Janon, Owen, etc.

Sobol' main indices: Rank statistics estimation

Pick-freeze approach:

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

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

for $j = 1{:}\,d$

for $i = 1{:}\,n$

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

$y_{ji} = f\left(z_1, \dots z_{j-1}, z_j, z_{j+1}, \dots z_d\right)$

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

Rank statistics approach*:

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

for $i = 1{:}\,n$

$y_i = f(z_1, \dots, z_d)$

for $j = 1{:}\,d$

$\hat{V}_j = \text{mean}_i\left(y_i y_{R_j(i)}\right) - \text{mean}_i(y_i)^2$

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:

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

and the ability to evaluate f at pick-freeze inputs

Rank statistics approach*:

requires n evaluations of f

at arbitrary i.i.d. inputs

*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

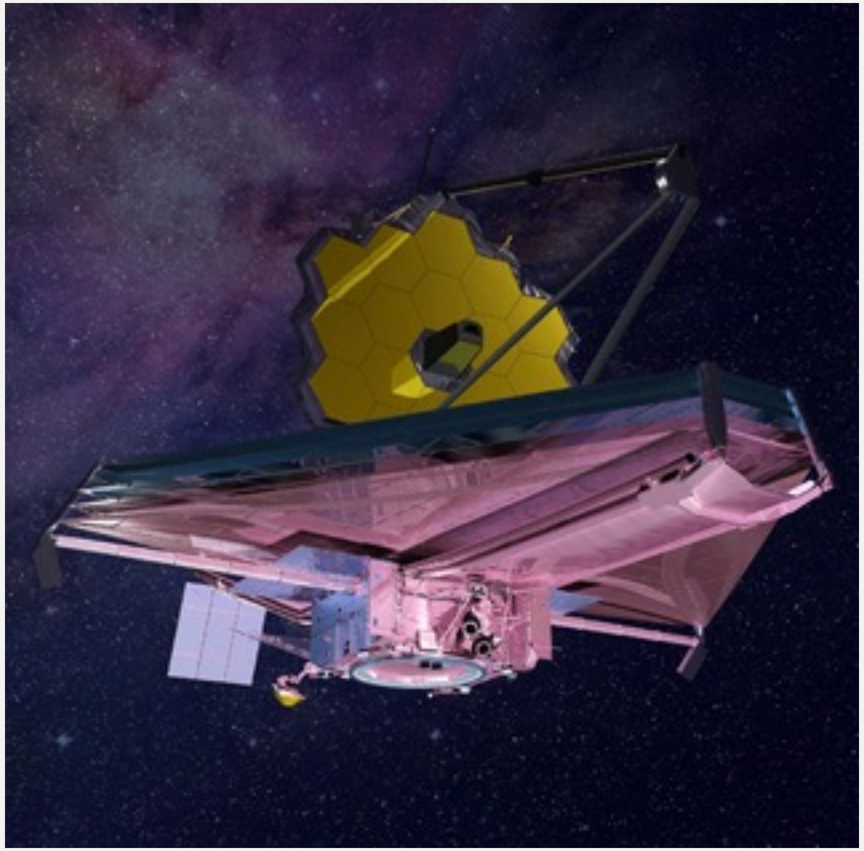
Motivating application: Space mission design

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:

$$\hat{\mu}_Y^N = \frac{1}{N}\sum_{i=1}^{N} y_i = \frac{1}{N}\sum_{i=1}^{N} f(z_i) \qquad \mathrm{Var}[\hat{\mu}_Y^N] = \frac{\mathrm{Var}[Y]}{N}$$

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

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

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

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

Variance reduction using control variates

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

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

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

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

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

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 $W = g(Z)$.

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

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

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

Multifidelity variance and Sobol estimators introduced in [2]

[1] Peherstorfer, Willcox, & Gunzburger CMAME 2016
[2] Q. et al. SIAM JUQ 2018

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 multi*level* 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

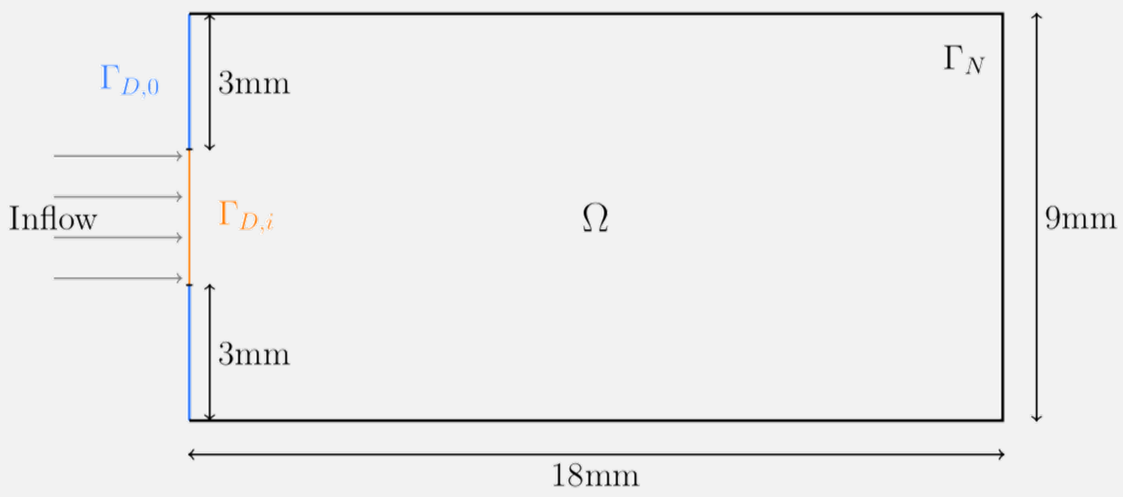
3. Numerical results
    - Convection-diffusion-reaction example
    - JWST wavefront error sensitivity

Example: 2D Convection-Diffusion-Reaction

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

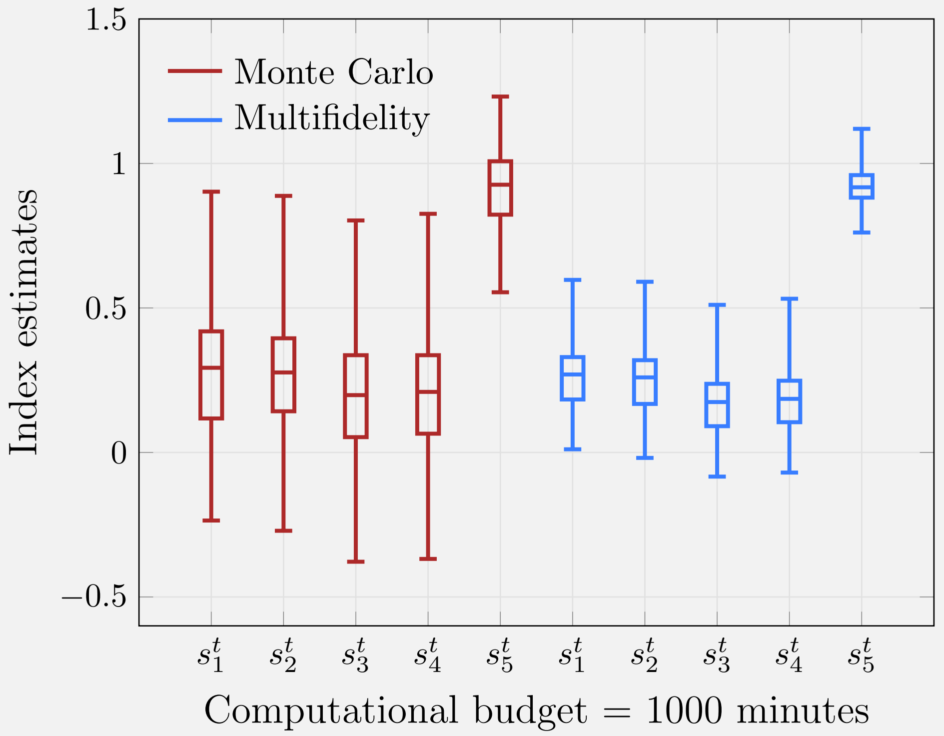
$$s_i(\mathbf{x}, \mathbf{p}) = \nu_i \left(\frac{W_i}{\rho}\right)\left(\frac{\rho Y_F}{W_F}\right)^{\nu_F}\left(\frac{\rho Y_O}{W_O}\right)^{\nu_O} A \exp\left(-\frac{E}{RT}\right), \ i = F, O, P,$$

$$s_T(\mathbf{x}, \mathbf{p}) = s_P(\mathbf{x}, \mathbf{p}) Q,$$

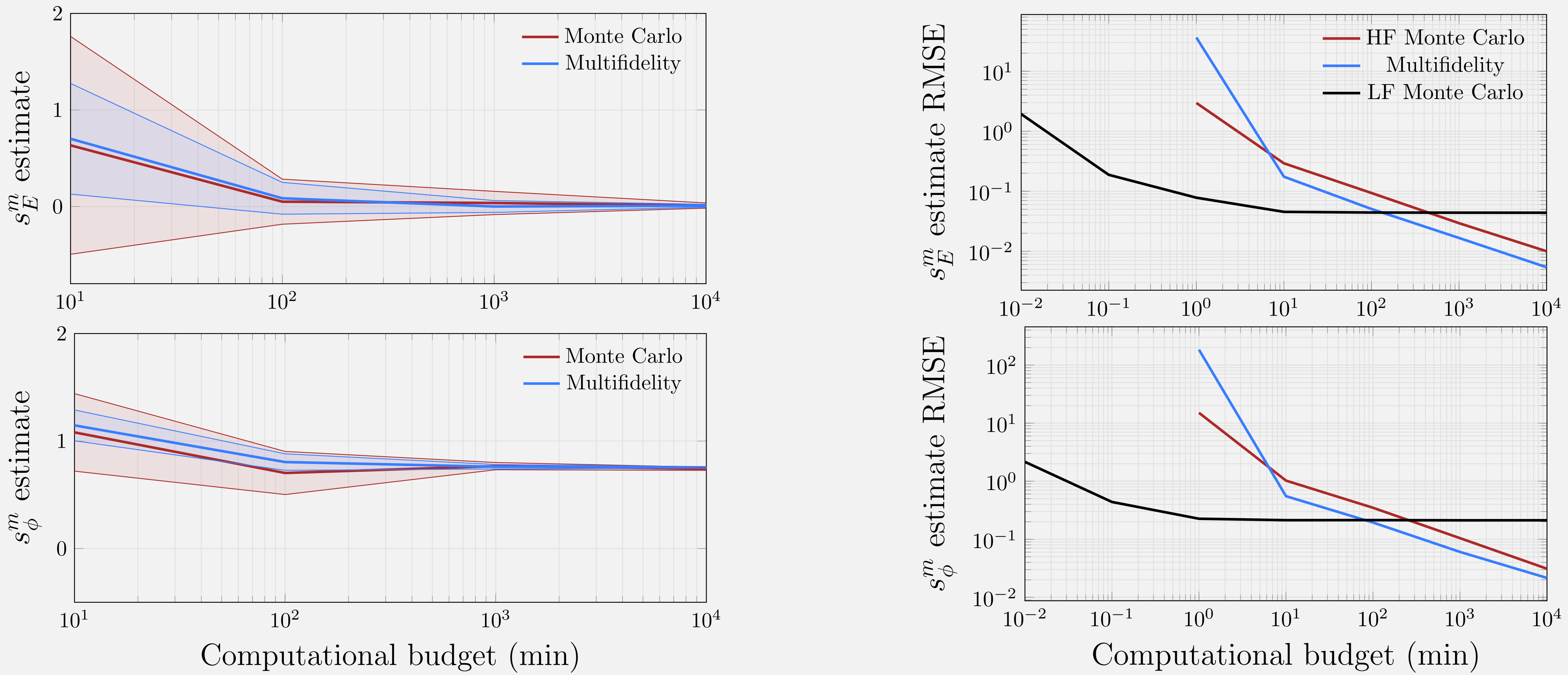


Uncertain parameters:

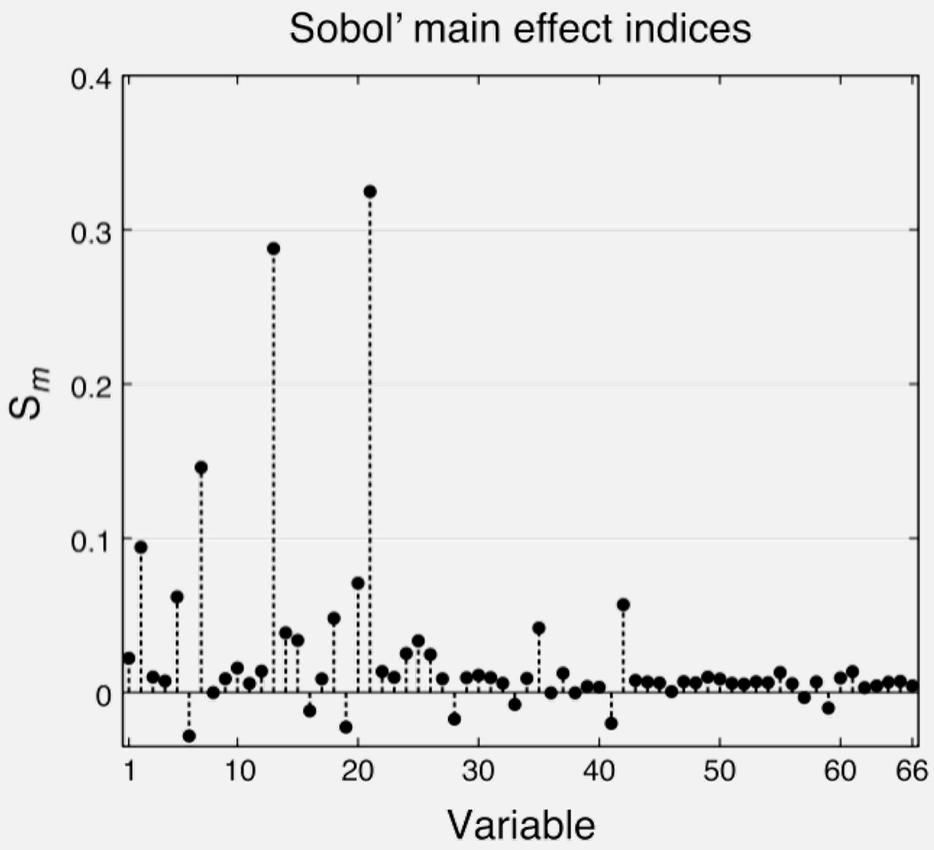
A, E, T_i, T_0, ϕ

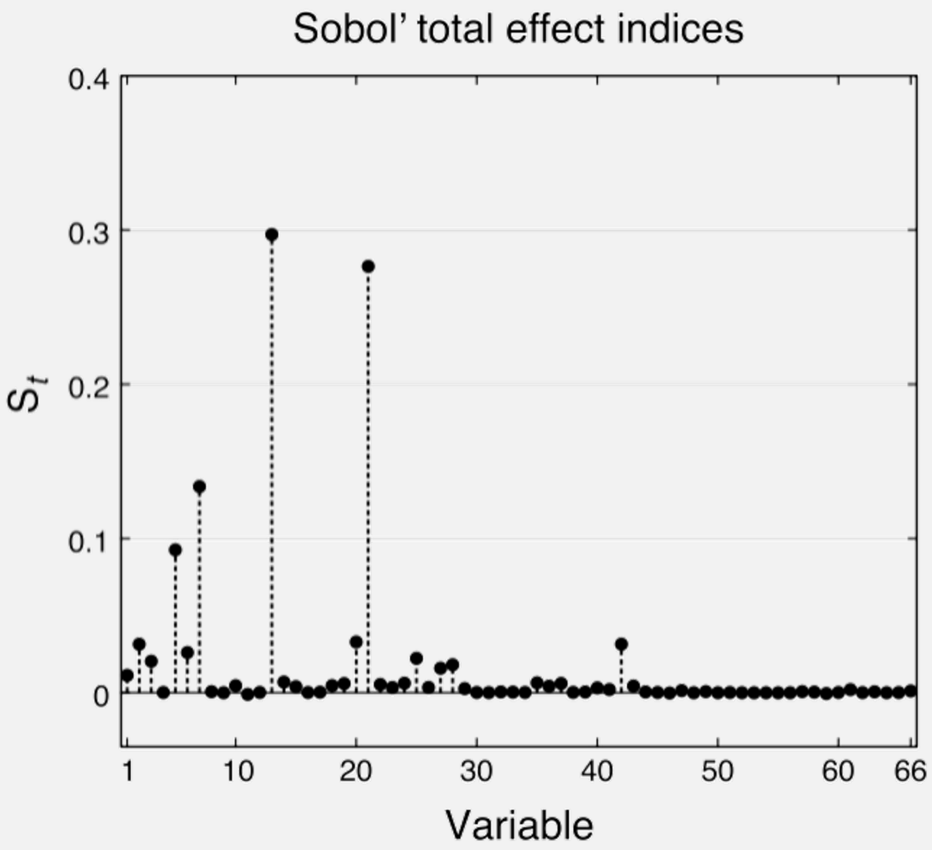


2D CDR Sobol' estimate convergence



JW Space Telescope revisited



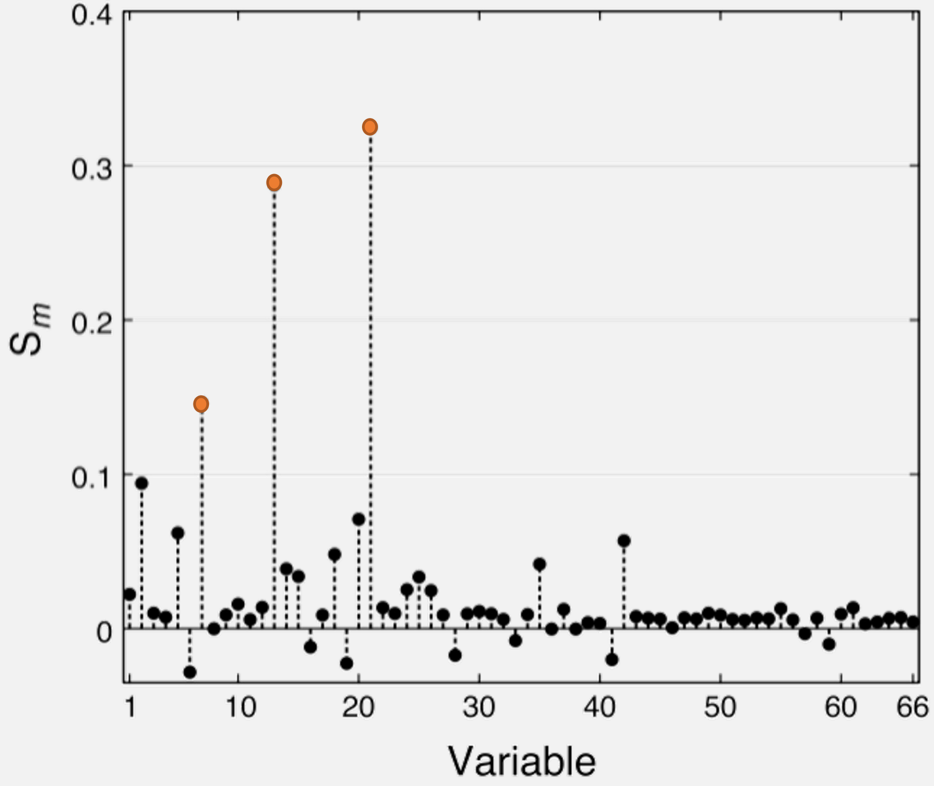


Multifidelity pick-freeze Sobol' estimators for JWST wavefront error with 60 day computational budget

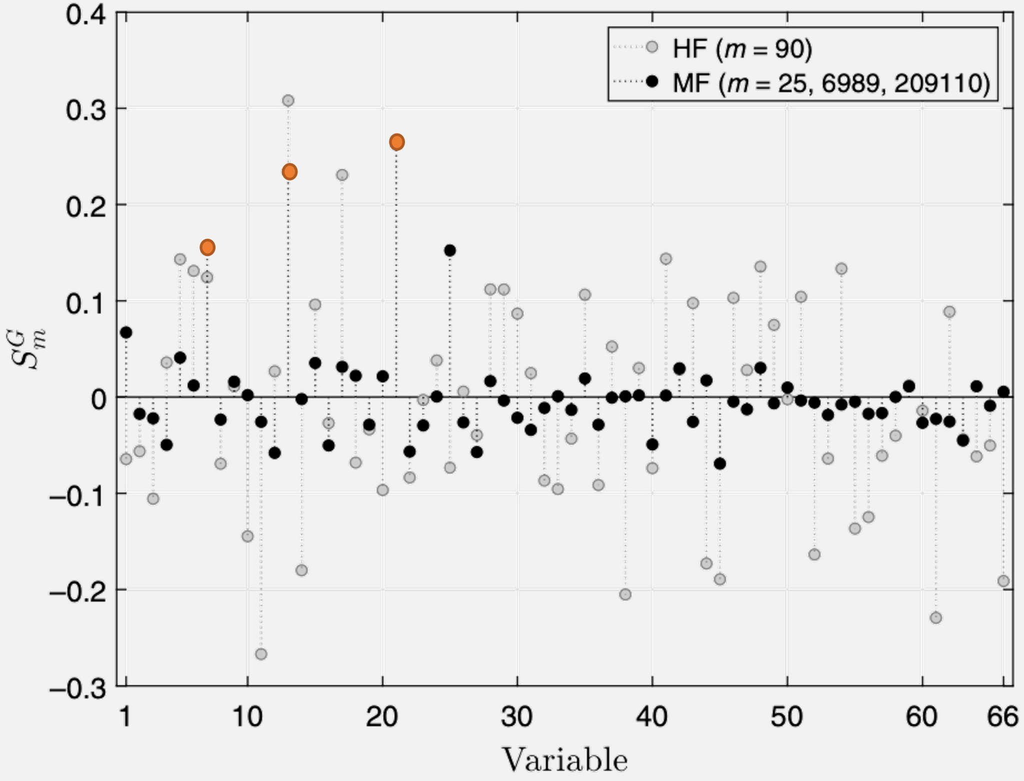
Multifidelity rank statistics estimators

Pick-Freeze

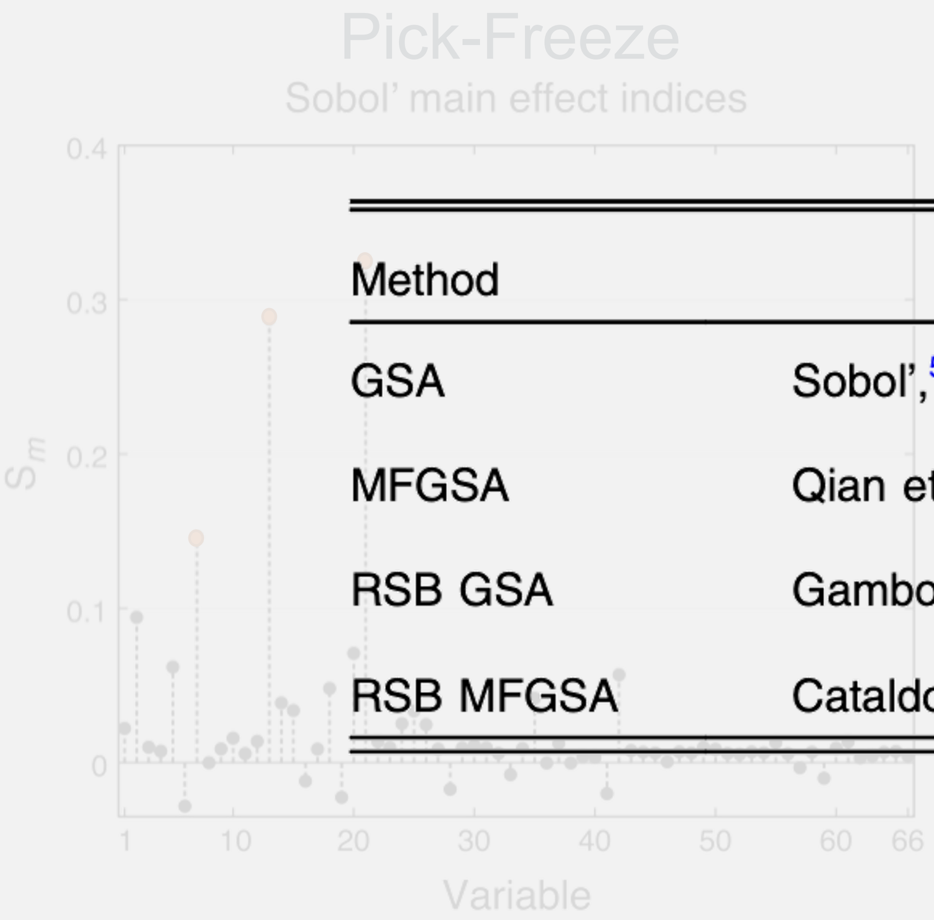
Sobol' main effect indices

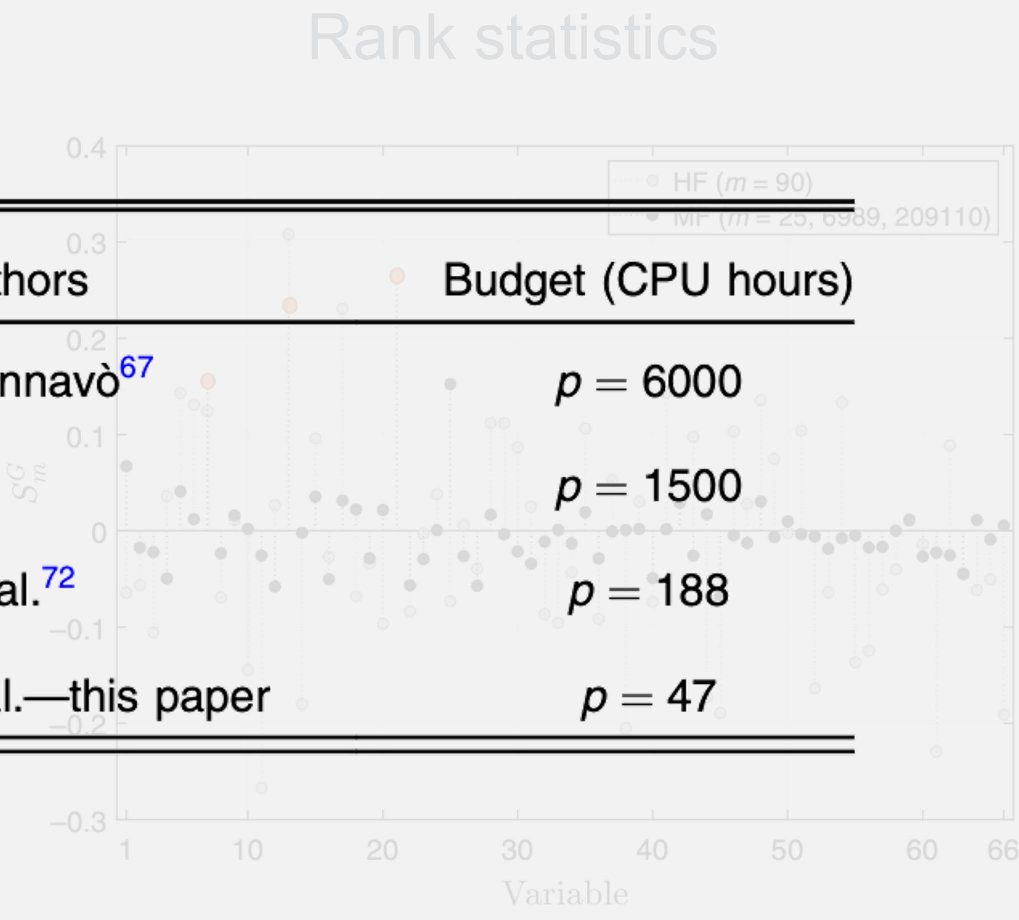


Rank statistics



Computational cost comparison





Method	Authors	Budget (CPU hours)
GSA	Sobol',[57] Cannavò[67]	$p = 6000$
MFGSA	Qian et al.[47]	$p = 1500$
RSB GSA	Gamboa et al.[72]	$p = 188$
RSB MFGSA	Cataldo et al.—this paper	$p = 47$

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 application

Thank you

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Papers:

- Qian, Peherstorfer, O’Malley, Vesselinov, and Willcox, SIAM Journal on Uncertainty Quantification, 2018.
- Cataldo, Qian, and Auclair, Journal of Astronomical Telescopes and Instrumentation Systems, 2022.
- Ask/email me if you’re interested in any of the other works I’ve mentioned

Github: elizqian/mfgsa