Minimizing the Number of Function Evaluations to Estimate Sobol' Indices Using Quasi-Monte Carlo

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Outline

- Introduction
  - ANOVA
  - Sobol' Indices
- Quasi-Monte Carlo Methods
- Replicated Method

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  - ANOVA—The ANalysis Of VAriance decomposition.
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ANOVA

For $f \in L^2\left([0,1]^d\right)$, and $\mathcal{D} = \{1, \dots, d\}$,

$$f(\boldsymbol{x}) = \sum_{u \subseteq \mathcal{D}} f_u(\boldsymbol{x}) \,, \qquad f_\varnothing = \mu \,,$$

where,

$$f_u(\boldsymbol{x}) = \int_{[0,1]^{d-|u|}} f(\boldsymbol{x}) d\boldsymbol{x}_{-u} - \sum_{v \subset u} f_v(\boldsymbol{x}) \,.$$

- $|u|$ the cardinality of u.
- $-u := u^c = \mathcal{D} \backslash u$.

Variance Decomposition

Under the previous definitions,

$$\sigma_{\varnothing}^2 = 0\,, \qquad \sigma_u^2 = \int_{[0,1]^d} f_u(\boldsymbol{x})^2 d\boldsymbol{x}\,, \qquad \sigma^2 = \int_{[0,1]^d} \left(f(\boldsymbol{x}) - \mu\right)^2 d\boldsymbol{x}\,.$$

The ANOVA identity is,

$$\sigma^2 = \sum_{u \subseteq \mathcal{D}} \sigma_u^2\,.$$

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  - Sobol' Indices—Measuring the importance of each input.
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Sobol' Indices

Sobol' introduced the *global sensitivity* indices which measure the variance explained by any dimension subset $u \in \mathcal{D}$:

$$\underline{\tau}_u^2 = \sum_{\substack{v \subseteq u \\ v \in \mathcal{D}}} \sigma_v^2 , \quad \text{and} \quad \overline{\tau}_u^2 = \sum_{\substack{v \cap u \neq \varnothing \\ v \in \mathcal{D}}} \sigma_v^2 .$$

We have the following properties,

- $\underline{\tau}_u^2 \leqslant \overline{\tau}_u^2$.
- $\underline{\tau}_u^2 + \overline{\tau}_{-u}^2 = \sigma^2$.

Sobol' Indices - Probabilistic Framework

For $\boldsymbol{X} \sim U[0,1]^d$, Sobol' indices can also be presented in the following form,

$$\underline{\tau}_u^2 = \mathrm{Var}\left[\mathbb{E}\left(f(\boldsymbol{X})|\boldsymbol{X}_u\right)\right] = \mathrm{Var}\left(f(\boldsymbol{X})\right) - \mathbb{E}\left[\mathrm{Var}\left(f(\boldsymbol{X})|\boldsymbol{X}_u\right)\right],$$

$$\overline{\tau}_u^2 = \mathrm{Var}\left(f(\boldsymbol{X})\right) - \mathrm{Var}\left[\mathbb{E}\left(f(\boldsymbol{X})|\boldsymbol{X}_{-u}\right)\right] = \mathbb{E}\left[\mathrm{Var}\left(f(\boldsymbol{X})|\boldsymbol{X}_{-u}\right)\right].$$

The Normalized Sobol' Indices

One may also use the normalized definition of the Sobol' indices,

$$S_u = \frac{\underline{\tau}_u^2}{\sigma^2} = \frac{\mathrm{Var}\left[\mathbb{E}\left(f(\boldsymbol{X})|\boldsymbol{X}_u\right)\right]}{\mathrm{Var}\left(f(\boldsymbol{X})\right)} = 1 - \frac{\mathbb{E}\left[\mathrm{Var}\left(f(\boldsymbol{X})|\boldsymbol{X}_u\right)\right]}{\mathrm{Var}\left(f(\boldsymbol{X})\right)},$$

$$S_u^{\text{tot}} = \frac{\overline{\tau}_u^2}{\sigma^2} = 1 - \frac{\mathrm{Var}\left[\mathbb{E}\left(f(\boldsymbol{X})|\boldsymbol{X}_{-u}\right)\right]}{\mathrm{Var}\left(f(\boldsymbol{X})\right)} = \frac{\mathbb{E}\left[\mathrm{Var}\left(f(\boldsymbol{X})|\boldsymbol{X}_{-u}\right)\right]}{\mathrm{Var}\left(f(\boldsymbol{X})\right)}.$$

satisfying $0 \leqslant S_u \leqslant S_u^{\text{tot}} \leqslant 1$.

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satisfying $0 \leqslant S_u \leqslant S_u^{\text{tot}} \leqslant 1$. More specifically, S_u is composed by,

$$S_u = 1 - \frac{I^{(1)}}{I^{(2)} - \left(I^{(3)}\right)^2}, \quad \text{where} \begin{cases} I^{(1)} \text{ is a } 2d - |u| \text{ dim. integral.} \\ I^{(2)} \text{ is a } d \text{ dim. integral.} \\ I^{(3)} \text{ is a } d \text{ dim. integral.} \end{cases}$$

Error bounds for S_u require more care than error bounds for $I^{(k)}$.

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Why Quasi-Monte Carlo?

To estimate S_u we need to approximate $I^{(1)}$, $I^{(2)}$, and $I^{(3)}$. However, in high dimensions we need a suitable technique:

Method	Convergence
Trapezoidal rule:	$\mathcal{O}(n^{-2/d})$
Simpson's rule:	$\mathcal{O}(n^{-4/d})$
IID Monte Carlo:	$\mathcal{O}(n^{-1/2})$
Quasi-Monte Carlo:	$\mathcal{O}(n^{-1+\varepsilon})$

(n: number of data points)

Estimating $I^{(1)}$, $I^{(2)}$, and $I^{(3)}$ automatically

Given ε_a and $\boldsymbol{x} \mapsto f(\boldsymbol{x})$, we want $\hat{I}$ such that

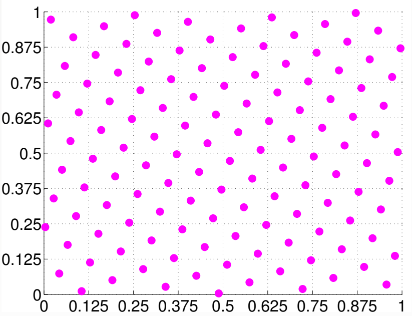
$$\left| \int_{[0,1)^d} f(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} - \hat{I}\left(\boldsymbol{x} \mapsto f(\boldsymbol{x}), \varepsilon_a\right) \right| \leqslant \varepsilon_a,$$

where

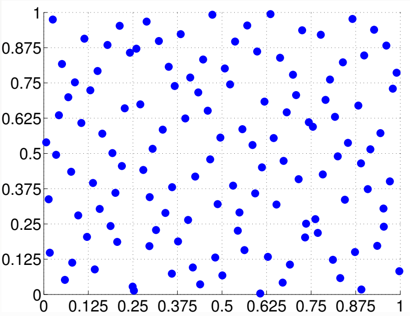
$$\hat{I}\left(\boldsymbol{x} \mapsto f(\boldsymbol{x}), \varepsilon_a\right) = \frac{1}{2^m} \sum_{i=0}^{2^m-1} f(\boldsymbol{z}_i),$$

for some automatic and adaptive choice of m and $\{\boldsymbol{z}_i\}_{i=0}^{\infty} \in \left\{ \begin{matrix} \text{Lattice} \\ \text{Digital} \end{matrix} \right\}$ sequence.

Examples of Sequences



Shifted rank-1 lattice sequence with generating vector $(1, 47)$.



Digitally shifted scrambled Sobol' sequence.

Outline

Normalized *First-Order* Sobol' Indices

In this particular case, we consider $|u| = 1$ and want to estimate $S_u = \sigma_u^2/\sigma^2$. For this purpose, given $\boldsymbol{x}, \boldsymbol{x}' \in [0,1]^d$, we define the following point,

$$(\boldsymbol{x}_u : \boldsymbol{x}'_{-u}) := (x'_1, \dots, x'_{u-1}, x_u, x'_{u+1}, \dots, x'_d) \in [0,1]^d.$$

Thus, one can use the following integral form to build an estimator:

$$S_u = 1 - \frac{\int_{[0,1)^{2d-1}} \overbrace{f(\boldsymbol{x})}^{g(\boldsymbol{x},\boldsymbol{x}'):=} \left(f(\boldsymbol{x}) - \overbrace{f(\boldsymbol{x}_u : \boldsymbol{x}'_{-u})}^{g_u(\boldsymbol{x},\boldsymbol{x}'):=}\right) d\boldsymbol{x} d\boldsymbol{x}'_{-u}}{\int_{[0,1]^d} f(\boldsymbol{x})^2 d\boldsymbol{x} - \left(\int_{[0,1]^d} f(\boldsymbol{x}) d\boldsymbol{x}\right)^2} = H(g, g_u)\,.$$

Number of Function Evaluations

We will focus on reducing the number of function evaluations, and to estimate σ_u^2/σ^2, only g and g_u are evaluated.

Computing all the indices one by one, if one requires n points for each estimation, the total number of function evaluations of g and g_u are

$$2dn\,,$$

However, if all indices are computed together, g only needs to be evaluated once. Therefore, the number of function evaluations becomes

$$(1+d)n\,,$$

Finally, under a special set of quasi-Monte Carlo sequences, this number is decreased to

$$2n\,.$$

Replicated Designs

Functions g and g_u only share input dimension u:

$$g(\boldsymbol{x}, \boldsymbol{x}') = f(x_1, \ldots, x_{u-1}, x_u, x_{u+1}, \ldots, x_d)\,,$$
$$g_u(\boldsymbol{x}, \boldsymbol{x}') = f(x'_1, \ldots, x'_{u-1}, x_u, x'_{u+1}, \ldots, x'_d)\,.$$

Hence, we can construct our points $\boldsymbol{x}'_i$ as follows,

$$\begin{pmatrix} x_{0,1} & \cdots & x_{0,d} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \cdots & x_{n,d} \\ \vdots & & \vdots \end{pmatrix}, \qquad \begin{pmatrix} x'_{0,1} & \cdots & x'_{0,d} \\ \vdots & \ddots & \vdots \\ x'_{n,1} & \cdots & x'_{n,d} \\ \vdots & & \vdots \end{pmatrix} = \begin{pmatrix} x_{\pi_1(0),1} & \cdots & x_{\pi_d(0),d} \\ \vdots & \ddots & \vdots \\ x_{\pi_1(n),1} & \cdots & x_{\pi_d(n),d} \\ \vdots & & \vdots \end{pmatrix}.$$

The Right Function Values

Given the right order of points:

$$\begin{pmatrix} \boldsymbol{x}'_{\pi_u^{-1}(0)} \\ \vdots \\ \boldsymbol{x}'_{\pi_u^{-1}(n)} \\ \vdots \end{pmatrix} = \begin{pmatrix} x'_{\pi_u^{-1}(0),1} & \cdots & x_{0,u} & \cdots & x'_{\pi_u^{-1}(0),d} \\ \vdots & & \vdots & & \vdots \\ x'_{\pi_u^{-1}(n),1} & \cdots & x_{n,u} & \cdots & x'_{\pi_u^{-1}(n),d} \\ \vdots & & \vdots & & \vdots \end{pmatrix}.$$

Therefore, we only need to evaluate $g_u(\boldsymbol{x}, \boldsymbol{x}')$ once:

$$\begin{pmatrix} f(\boldsymbol{x}'_0) \\ \vdots \\ f(\boldsymbol{x}'_n) \\ \vdots \end{pmatrix} = \begin{pmatrix} y_0 \\ \vdots \\ y_n \\ \vdots \end{pmatrix} \Longrightarrow \begin{pmatrix} g_u(\boldsymbol{x}_0, \boldsymbol{x}'_0) \\ \vdots \\ g_u(\boldsymbol{x}_n, \boldsymbol{x}'_n) \\ \vdots \end{pmatrix} = \begin{pmatrix} y_{\pi_u^{-1}(0)} \\ \vdots \\ y_{\pi_u^{-1}(n)} \\ \vdots \end{pmatrix}$$

Conclusions

- We can study how each dimension explains the overall variance of a model using Sobol' Indices.
- Our quasi-Monte Carlo automatic cubatures can be adapted to estimate these indices automatically.
- *First-order* Sobol' Indices can be estimated using only $2n$ quasi-Monte Carlo function evaluations (not depending on d).

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