Automatic estimation of Sobol' indices based on quasi-Monte Carlo methods

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Outline

- Introduction
- Sobol' Indices
- Quasi-Monte Carlo Methods
- Numerical example

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ANOVA

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

$$f(\boldsymbol{x}) = \sum_{u \subseteq 1:d} f_u(\boldsymbol{x})\,, \qquad f_\varnothing = \mu\,,$$

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.
- $-u := u^c$.

Variance Decomposition

Under the previous definitions,

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

The ANOVA identity is,

$$\sigma^2 = \sum_{u \subseteq 1:d} \sigma_u^2\,.$$

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Sobol' Indices for Uncertainty Quantification

We consider the random variable $Y = f(\boldsymbol{X})$ with $\boldsymbol{X} \sim U\left([0,1)^d\right)$.

Sobol' introduced the *global sensitivity* indices which measure the variance explained by any dimension subset $u \subseteq 1:d$:

$$\underline{\tau}_u^2 = \sum_{\substack{v \subseteq u \\ v \subseteq 1:d}} \sigma_v^2 \,, \qquad \text{and} \qquad \overline{\tau}_u^2 = \sum_{\substack{v \cap u \neq \varnothing \\ v \subseteq 1:d}} \sigma_v^2 \,.$$

We have the following properties,

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

Estimation of the Integral

Indices $\underline{\tau}_u^2$ and $\overline{\tau}_u^2$ can be estimated with integrals:

$$\underline{\tau}_u^2 = \int_{[0,1]^{2d-1}} f(\boldsymbol{x}) f(\boldsymbol{x}_u : \boldsymbol{x'}_{-u}) d\boldsymbol{x} d\boldsymbol{x'} - \left(\int_{[0,1]^d} f(\boldsymbol{x}) d\boldsymbol{x} \right)^2,$$

$$\overline{\tau}_u^2 = \frac{1}{2} \int_{[0,1]^{d+1}} \left(f(\boldsymbol{x'}) - f(\boldsymbol{x}_u : \boldsymbol{x'}_{-u}) \right)^2 d\boldsymbol{x} d\boldsymbol{x'}.$$

where the point $\boldsymbol{z} := (\boldsymbol{x}_u : \boldsymbol{x'}_{-u})$ has coordinates $z_j = x_j$ if $j \in u$, and $z_j = x'_j$ if $j \notin u$.

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- Quasi-Monte Carlo Methods—How can we estimate integrals in high dimensions?
- Numerical example

Numerical Integration Problem

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

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

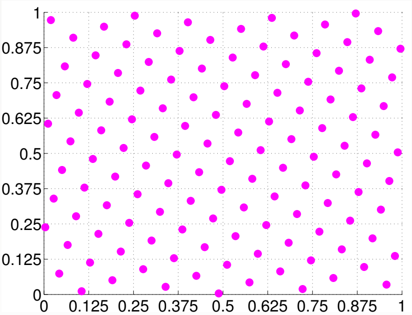
where

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

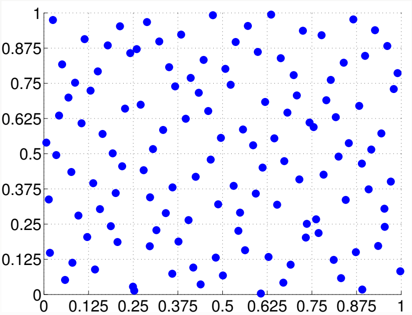
for some automatic and adaptive choice of m, $\{\boldsymbol{z}_i\}_{i=0}^{\infty} \in \left\{\begin{matrix}\text{Lattice} \\ \text{Digital}\end{matrix}\right\}$ sequence, and

$$\mathrm{cost}\left(\hat{I}\left(\boldsymbol{x} \mapsto f(\boldsymbol{x}), \varepsilon_a\right)\right) = \mathcal{O}\left((m + \$(f))2^m\right)$$

Examples of Sequences



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



Digitally shifted scrambled Sobol' sequence.

Adaptive Algorithm

The idea behind the results in Jiménez Rugama and Hickernell (2016+) and Hickernell and Jiménez Rugama (2016+) is that for all $f \in \mathcal{C}$,

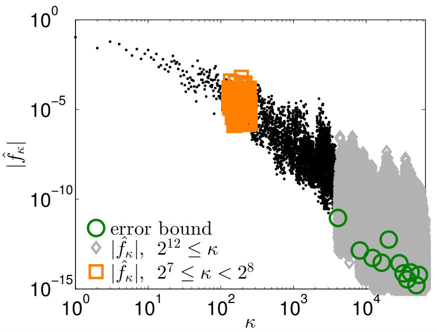
$$\left| \int_{[0,1)^d} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} - \hat{I}\left(\boldsymbol{x} \mapsto f(\boldsymbol{x}), \varepsilon_a\right) \right| \leqslant a(r,m) \sum_{\kappa=\lfloor 2^{m-r-1} \rfloor}^{2^{m-r}-1} \left| \tilde{f}_{m,\kappa} \right|.$$

- $\tilde{f}_{m,\kappa}$ = discrete Fourier $\left\{ \begin{matrix} \text{Exponential} \\ \text{Walsh} \end{matrix} \right\}$ coefficients of f.
- $a(r,m)$ = inflation factor that depends on $\mathcal{C}$.

QMC Error Bounds Depend Only on Some Fourier Coefficients for $f \in \mathcal{C}$

In the quasi-Monte Carlo case,

$$\left| I(f) - \frac{1}{2^m} \sum_{i=0}^{2^m-1} f(\boldsymbol{z}_i \oplus \boldsymbol{\Delta}) \right| \leqslant \sum \bigcirc \leqslant a(r,m) \sum_{\kappa=\lfloor 2^{m-r-1} \rfloor}^{2^{m-r}-1} \left| \tilde{f}_{m,\kappa} \right|$$



$$\mathcal{C} = \left\{ \sum \square \text{ bounds } \sum \lozenge \atop \sum \lozenge \text{ bounds } \sum \bigcirc \right\}$$

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- Numerical example—The Bratley et al. (1992) function

Bratley et al. (1992)

$$f(\boldsymbol{X}) = \sum_{i=1}^{6} (-1)^i \prod_{j=1}^{i} \boldsymbol{X}_j = -\boldsymbol{X}_1 + \boldsymbol{X}_1\boldsymbol{X}_2 - \boldsymbol{X}_1\boldsymbol{X}_2\boldsymbol{X}_3 + \ldots$$

Values	$j=1$	$j=2$	$j=3$	$j=4$	$j=5$	$j=6$
S_j	65.3%	17.9%	3.7%	1.3%	0.1%	0.1%
S_j^{tot}	74.0%	26.6%	7.7%	3.3%	0.6%	0.7%

n	$j=1$	$j=2$	$j=3$	$j=4$	$j=5$	$j=6$
S_j	65536	32768	16384	8192	2048	1024
S_j^{tot}	32768	16384	8192	4096	1024	1024

Computation time was 0.37 seconds for $\varepsilon_a = 10^{-3}$.

Conclusions and Future Work

- The Sobol' indices algorithm accepts user input relative error tolerances.
- The estimation can be performed over the normalized indices.
- First-order indices can also be estimated using the replicated method because quasi-Monte Carlo methods are compatible with the replicated method.

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Inside and Outside $\mathcal{C}$