Referee report on
"Reliable error estimation for Sobol' indices"
by Rugama and Gilquin

Overview

Sobol' indices are used to measure variable importance. They involve expensive integrals. This paper applies recent developments in integration subject to given error bounds to the problem of estimating Sobol' indices.

Larger points

1. Definition 1 is not enough to get good points. Additional criteria should be attached to it, either by making the definition stricter or requiring some other conditions to hold.

   To illustrate, suppose that $u_0, \ldots, u_{n-1} \in [0,1]$ are chosen. Then let $\boldsymbol{x}_i = (u_i, u_i, \ldots, u_i) \in \mathbb{R}^d$ and choose $\boldsymbol{x}'_i = \boldsymbol{x}_{\pi(i)}$ where π is a permutation of 0 through $n-1$. Now we have replicated designs of order a for any $a = 1, \ldots, d-1$. In fact simply taking $n = 1$ and $\boldsymbol{x}' = \boldsymbol{x} \in [0,1]^d$ will do.

   Also, how is π_u defined when there is more than one permutation that rearranges the rows $\boldsymbol{x}'_i$ into $\boldsymbol{x}_i$? Maybe it should say "to be any permutation that rearranges the rows ...".

2. Section 3.1 needs more detail for readers not already familiar with the approach. For instance on page 4 line 16 a little should be said about what $k_{j\ell}$ is. It should also briefly say in words what S_m, $\widehat{S}_{\ell,m}$, $\check{S}_m$, and $\tilde{S}_{\ell,m}$ all mean.

3. Page 5 line 56 presents some bounds that the Sobol' indices must satisfy. Sometimes they won't satisfy those bounds. When do they fail, how that be detectable, and what can we do in the face of bounds that might or might not hold? Presumably these issues have been discussed in simpler contexts. The paper should address this issue.

4. If we replace f by $f - c$ for some constant shift c, then the Sobol' indices do not change. But the bounds for $\underline{S}_u$ and $\overline{S}_u$ do change because $\mathbf{I}_3$ is affected. What could/should we do about this?

5. Page 7 lines 22:27. The discussion here is saying that the higher dimensional integrand is likely to be the one that needs more evaluations. That is not in line with the last couple of decades of QMC theory. The nominal dimension might not be very telling. Maybe only a few of the inputs are important in the higher dimensional integrand, or maybe the higher order variable interactions are less important for that integrand.

So, can you give a better reason for why that integrand might need larger n? Alternatively, in the numerical examples, which integrands required the most evaluations?

(This point touches on the circular issue, perhaps best avoided, of finding which variables are important when you're estimating a Sobol' index.)

6. In Section 5.1.1, the Sobol' g-function looks like a potentially misleading choice. It is completely smooth except when one of the inputs is 1/2. That makes it a particularly favorable problem for Sobol' points or any points in base 2. The problem might just be too QMC-friendly. It would be better to use $g_j(x_j) = (|3x_j - 2| + a_j)/(1 + a_j)$ which has issues when $x_j = 2/3$ which is not dyadic. The QMC friendly version might still work exactly the same as the unfriendly version, but changing g just removes that issue from consideration.

7. The Asian option is very over used in QMC problems. We already know that BB and PC make the first component most important. It might be interesting to compare these two, although the answer might depend on the strike price and volatility.

   For the same amount of work, the authors could use a real function where the answer would be interesting. Derek Bingham maintains a site of test functions for computer experiments. Some of those would be more suitable.

8. Sobol' indices are often motivated by the need to identify important variables when f is expensive to evaluate; perhaps half a day for $n = 1$. Estimates that require n to be several hundred thousand do not fit that motivating context. If the authors can describe a context where it would be worth having $n = 400{,}000$ to get a Sobol' estimate, that would be great. Nobody else has properly addressed this issue, so this point is a suggestion, not a requirement.

Smaller points

1. page 2 line 48: it should be clear that $v \subset u$ excludes $v = u$.

2. page 2 line 59: it is not clear why $u = \mathcal{D}$ is ruled out. In that case both $\overline{\tau}_u^2$ and $\underline{\tau}_u^2$ equal σ^2.

3. equation (7) is a numerically poor way to estimate σ^2 (roundoff errors).

4. page 3 line 37: accordingly $\rightarrow$ according

5. page 4: there is a symbol class of S for Sobol' indices with $S_m(f)$ and related quantities. The paper could note the distinction or possibly use a new letter.

6. page 8 line 16: twice as small $\rightarrow$ half as large