Method-independent, Computationally Frugal Convergence Testing for Sensitivity Analyses

J. Mai [1] and B. Tolson [1]

[1] University of Waterloo, Waterloo, Canada   Contact: (juliane.mai@uwaterloo.ca)

1. Introduction

The increasing complexity and runtime of environmental models lead to the current situation that the calibration of all model variables or the estimation of all of their uncertainty is often computationally infeasible. Hence, techniques to determine the sensitivity of model variables are used to **identify most important variables** or model processes. While the examination of the convergence of calibration and uncertainty methods is state-of-the-art, the **convergence of sensitivity analyses (SA) results is usually not checked**. If any, bootstrapping of the sensitivity results is used to determine the reliability of estimated indexes. Bootstrapping, however, requires non-negligible implementation efforts and can also become computationally expensive in case of large model outputs and a high number of bootstraps. It also does not perform well for small sample sizes. We, therefore, present a **Model Variable Augmentation (MVA)** approach for improved interpretation of SA experiments. MVA is:

- method- and model independent
- computationally frugal
- applicable during or after the SA

2. Test functions & Experimental Setup

The method is tested using the methods of **Sobol' sensitivity indexes** (Sobol', 1993) and the **PAWN indexes** (Pianosi & Wagener, 2015). Different numbers of variable sets N_S (a proxy for number of model runs) were used, i.e. 10, 100, and 1000. To compare the results of MVA with standard approaches the indexes were also bootstrapped. The number of bootstrap samples was set to $N_B = 1000$. We employed 12 benchmark functions with different numbers of variables N_X to demonstrate the reliability of MVA.

$f(x)$	N_X	Distr. x_i	μ_f	σ_f^2	var. with import. low	interm.	high
Sobol's G	6	$\mathcal{U}[0,1]$	1.0	0.2	4	1	1
Saltelli's G_1^*	10	$\mathcal{U}[0,1]$	1.0	0.8	8	0	2
Saltelli's G_2^*	10	$\mathcal{U}[0,1]$	1.0	3.0	6	4	0
Saltelli's G_3^*	10	$\mathcal{U}[0,1]$	1.0	0.3	8	0	2
Saltelli's G_4^*	10	$\mathcal{U}[0,1]$	1.0	0.7	8	2	0
Saltelli's G_5^*	10	$\mathcal{U}[0,1]$	1.0	2.5	8	0	2
Saltelli's G_6^*	10	$\mathcal{U}[0,1]$	1.0	20.0	4	6	0
Bratley's K	10	$\mathcal{U}[0,1]$	-0.3	0.1	8	1	1
Saltelli's B	10	$\mathcal{N}[0,\sigma]$	0.0	2.0	6	4	0
Ishigami-H.	3	$\mathcal{U}[-\pi,\pi]$	1.0	2100.0	1	0	2
Oakley-O'H.	15	$\mathcal{N}[0,1]$	11.0	37.0	15	0	0
Morris	20	$\mathcal{U}[0,1]$	30.0	1100.0	10	5	5

3. Model Variable Augmentation MVA

- augment true model with artificial model variables z_0, z_1, and z_2 with known properties
- original model output $f(x)$ is converted into $y(x,z,c)$ where c is a correction factor such that $\sigma_f^2 \equiv \sigma_y^2$
- S_i describes the sensitivity of parameter i
- z_0 is dummy variable to check correctness of sensitivity method itself ($S_{z_0} = 0$)
- z_1 and z_2 are variables which variances are controlled by a SA index specific parameter Δ to check for sampling uncertainty ($S_{z_1} = S_{z_2}$)

	Bootstrapping	MVA
Convergence	Analyze mean $\mu^{(B)}$ and variance $\sigma^{(B)}$ of bootstrapped distribution $\mathcal{D}^{(B)}$ of sensitivity indexes. Convergence, if rel. error is below δ_C: $\frac{\mu_i^{(B)}}{\sigma_i^{(B)}} < \delta_C \; \forall x_i$	Determine number of variables with sensitivity between sensitivities of augmented variables z_1 and z_2. No evidence of non-convergence if: $S_{z_1} < S_{x_i} < S_{z_2} \; \nexists x_i$
Screening	Identify variables above certain threshold δ_B as important: $S_i > \delta_B$	Identify variables above certain threshold δ_M as important: $S_i > \delta_M$ with $\delta_M = \delta_B - \lvert S_{z_1} - S_{z_2} \rvert$
Ranking	Kolmogorov-Schmirnov test to check if bootstrap distributions of sensitivity indexes for two variables x_i and x_j are significantly different: $\mathcal{H}_0: \mathcal{D}_{S_i}^{(B)} = \mathcal{D}_{S_j}^{(B)}$	Check if difference between indexes of two variables S_i and S_j is smaller than difference for augmented variables z_1 and z_2. Variables are indistinguishable if: $\lvert S_i - S_j \rvert \leq \lvert S_{z_1} - S_{z_2} \rvert$

5. Conclusions

- MVA is computationally **less expensive** than bootstrapping since automatically computed during sens. estimation
- MVA indicates **reliability** of sens. estimates (Fig. 1 & 2)
- MVA allows for **seamless check** of certainty of SA results
- MVA identifies **important variables** more reliably than standard fixed-threshold method (Fig. 6)

4. Results

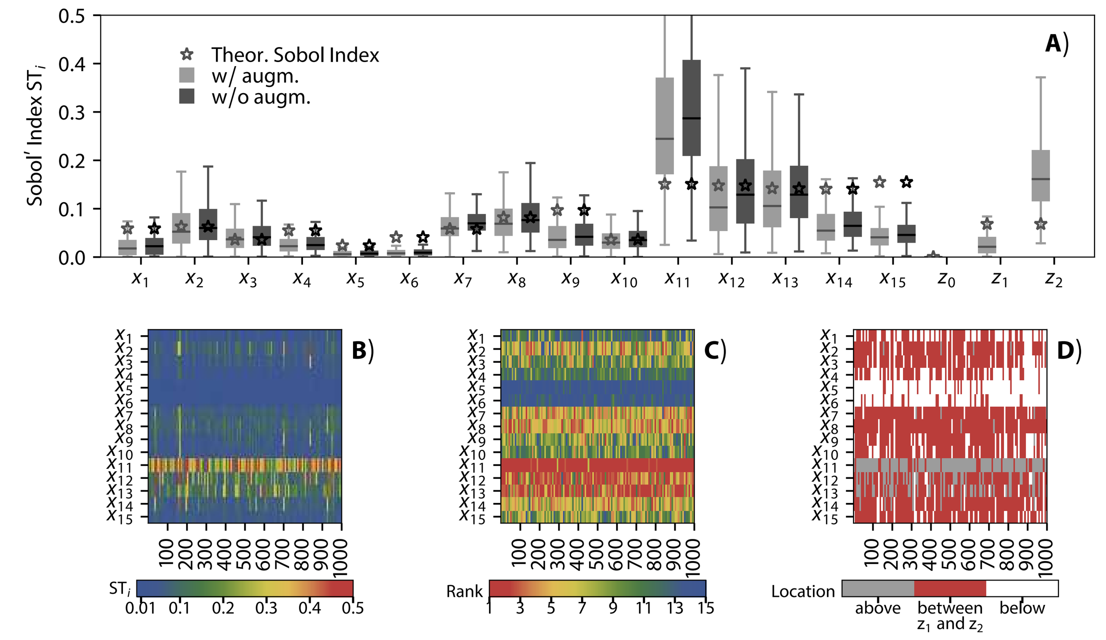

Fig. 1: Results of a **Sobol' sensitivity analysis** for the Oakley-O'Hagan test function using **10 variable sets** and a confidence threshold Δ of 0.2. (A) shows the Sobol' sensitivity indexes with and without MVA as well as the true Sobol indexes. In (B) the individual indexes of all 1000 bootstraps and in (C) the ranking of the variables is depicted. (D) shows how many variables are enveloped by the augmented variables (red) and hence are not converged.

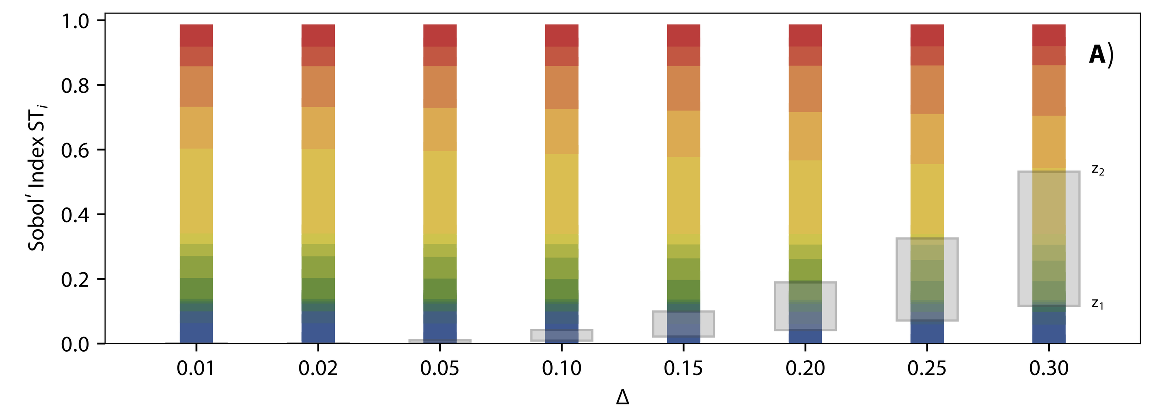

Fig. 4: **Sobol' indexes** of the dummy parameters z_1 and z_2 (gray box) relative to the other parameter sensitivities of the Oakley-O'Hagan test function using **10 variable sets** and no bootstrap. Color indicates the parameter index i.

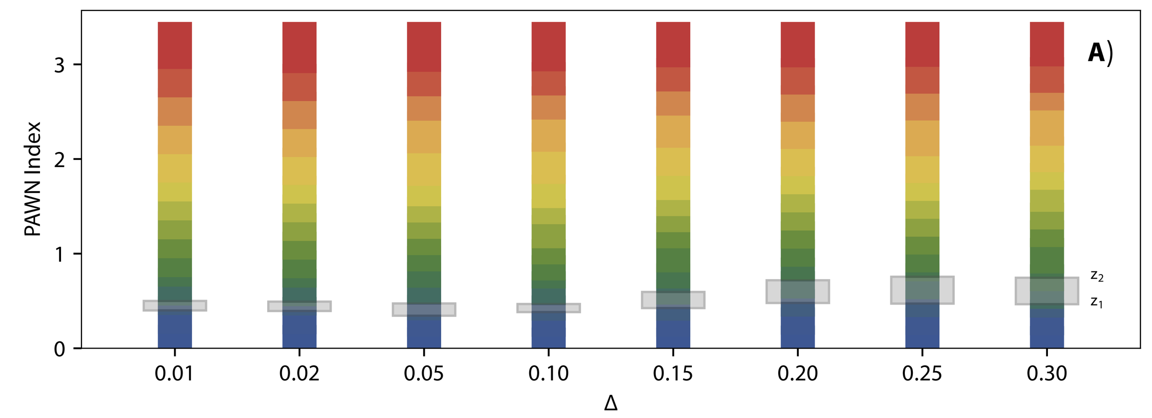

Fig. 5: **PAWN indexes** of the dummy parameters z_1 and z_2 (gray box) relative to the other parameter sensitivities of the Oakley-O'Hagan test function using **10 variable sets** and no bootstrap.

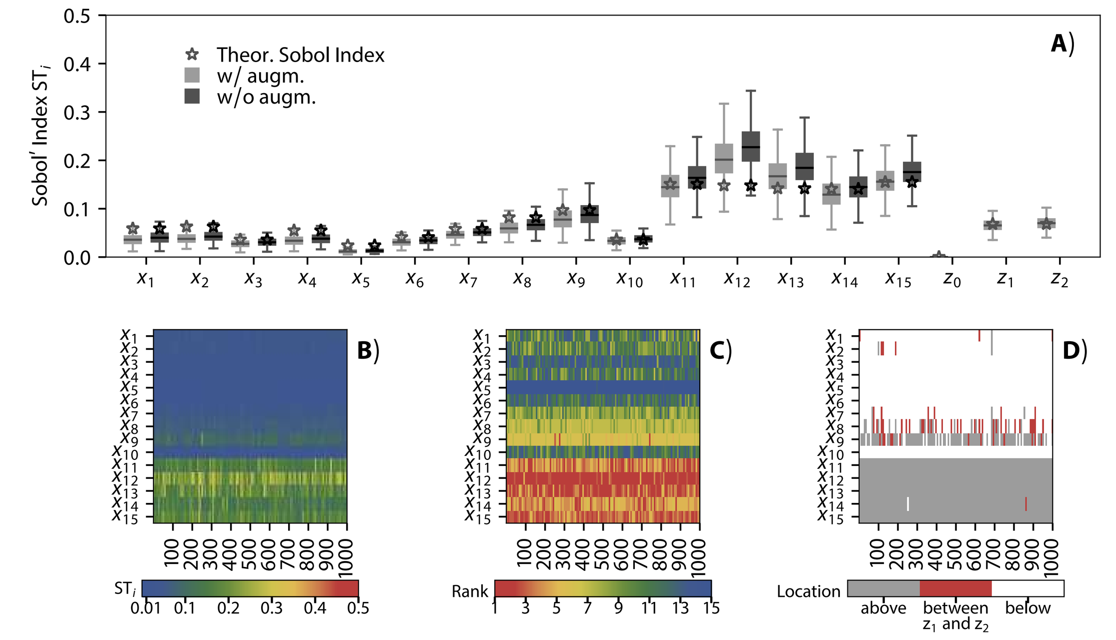

Fig. 2: Results of a **Sobol' sens. analysis** for the Oakley-O'Hagan test function using **100 variable sets** and a confidence threshold Δ of 0.2. The subplots are the same as in Figure 1.

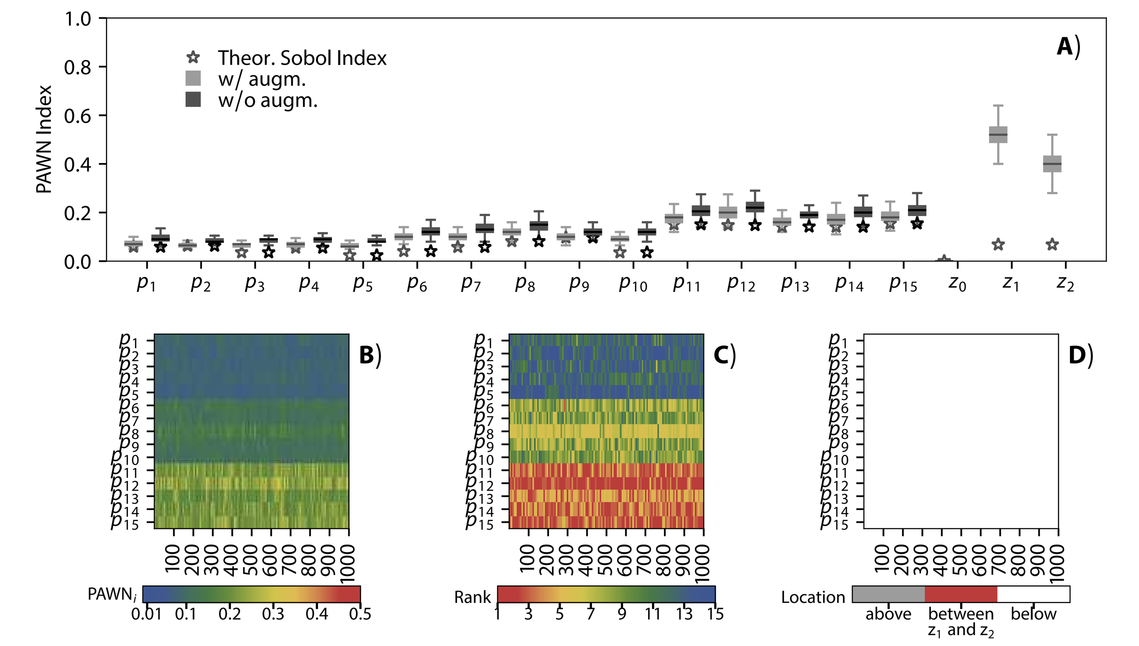

Fig. 3: Results of a **PAWN sensitivity analysis** for the Oakley-O'Hagan test function using **100 variable sets** and a confidence threshold Δ of 0.2. The individual subplots are the same as in Figure 1.

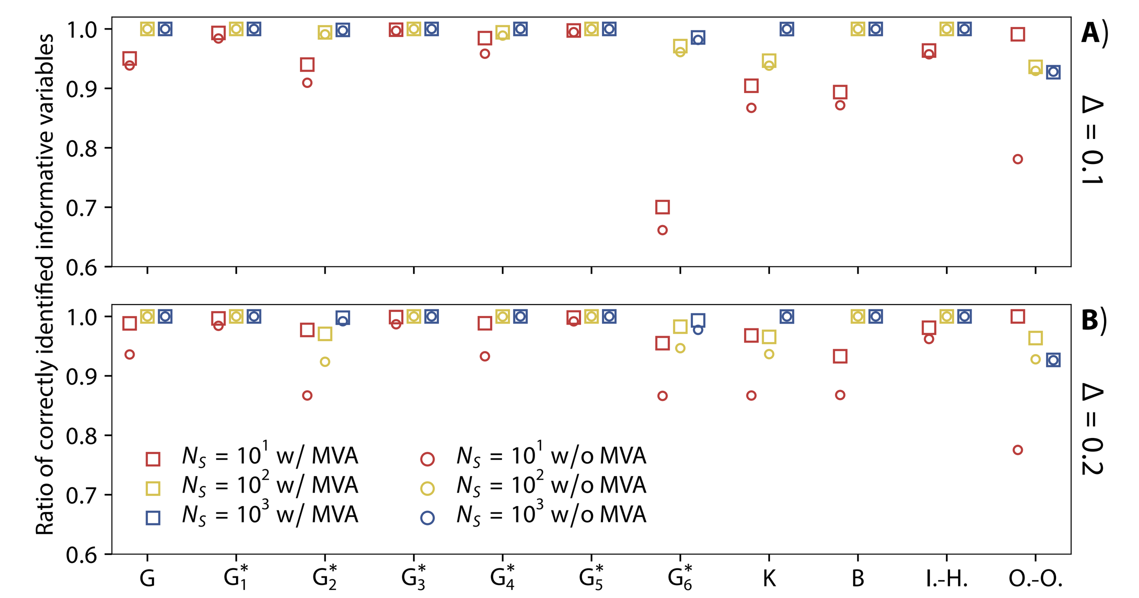

Fig. 6: Ratio of correctly determined informative variables using different confidence thresholds Δ and different numbers of reference sets N_S used to estimate the **Sobol' sensitivities**. The variable augmentation MVA is increasing the number of correctly identified informative variables in all experiments (compare squares and circles).