# Method-independent, Computationally Frugal Convergence Testing for Sensitivity Analyses

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## 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 the sensitivity methods is usually not checked**. If any, bootstrapping of the sensitivity results is used to determine the reliability of the 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 to check the convergence of sensitivity indexes without performing any additional model run. This technique is **method- and model-independent**. It can be applied either during the sensitivity analysis (SA) or afterwards.

## 2. Test functions & Experimental Setup

The method is tested using the variance-based, global method of Sobol' sensitivity indexes. Different numbers of reference variable sets $N_S$ were used, i.e. $10$, $100$, and $1000$. To compare the results of MVA with standard approaches the sensitivity 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 $N_X$ presented already in several studies such as Cuntz et. al (2016) to demonstrate the reliability of MVA.

| $f(x)$ | $N_X$ | Distr. $x_i$ | $\mu_f$ | $\sigma_f^2$ | 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 $\sigma_f^2 \equiv \sigma_y^2$
- $z_0$ is dummy variables to check correctness of sensitivity method itself ($S_{z_0} = 0$)
- $z_1$ and $z_2$ are variables which variance is controlled by parameter $\Delta$ 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 $\delta_C$: $\frac{\mu_i^{(B)}}{\sigma_i^{(B)}} < \delta_C \; \forall x_i$ | 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 $\delta_B$ as important: $S_i > \delta_B$ | Identify variables above certain threshold $\delta_M$ as important: $S_i > \delta_M = \delta_B - \lvert S_{z_1} - S_{z_2} \rvert$ |
| 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 indicates **non-converged** sens. estimates (Fig. 3)
- MVA identifies **indistinguishable variables** (Fig. 4)
- MVA identifies **important variables** more reliably than standard fixed-threshold method (Fig. 5)

## 4. Results

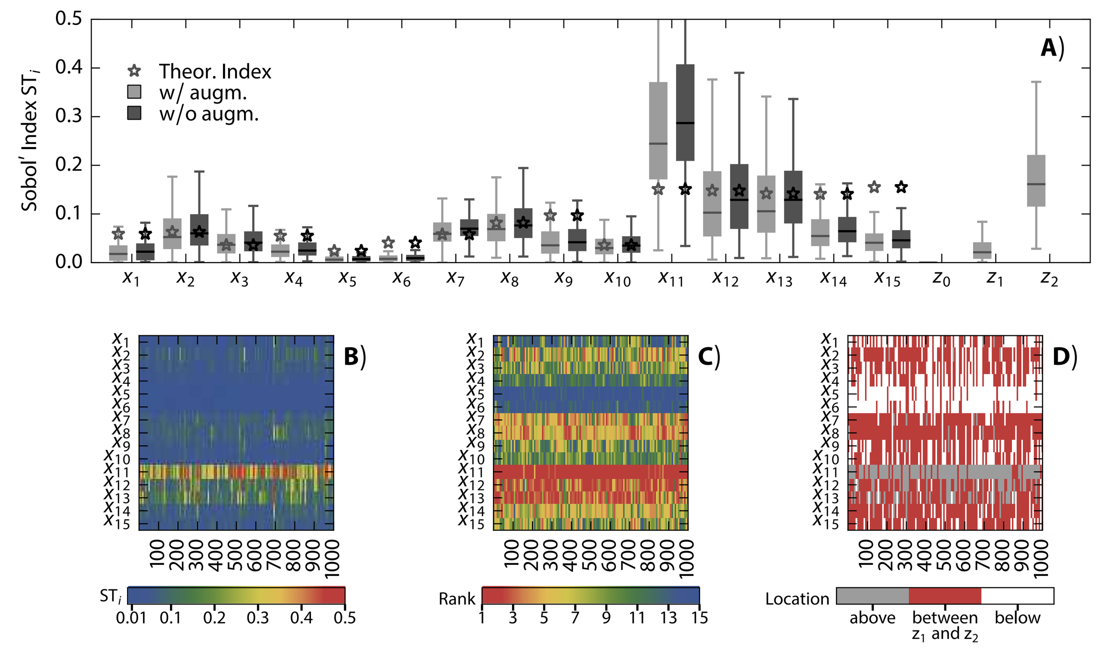


**Fig. 1:** Results of a Sobol' sensitivity analysis for the Oakley-O'Hagan test function using 10 reference variable sets and a confidence threshold $\Delta$ of 0.2. (A) shows the Sobol' sensitivity indexes with and without MVA as well as the true indexes. In (B) the individual indexes of all 1000 bootstraps 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.

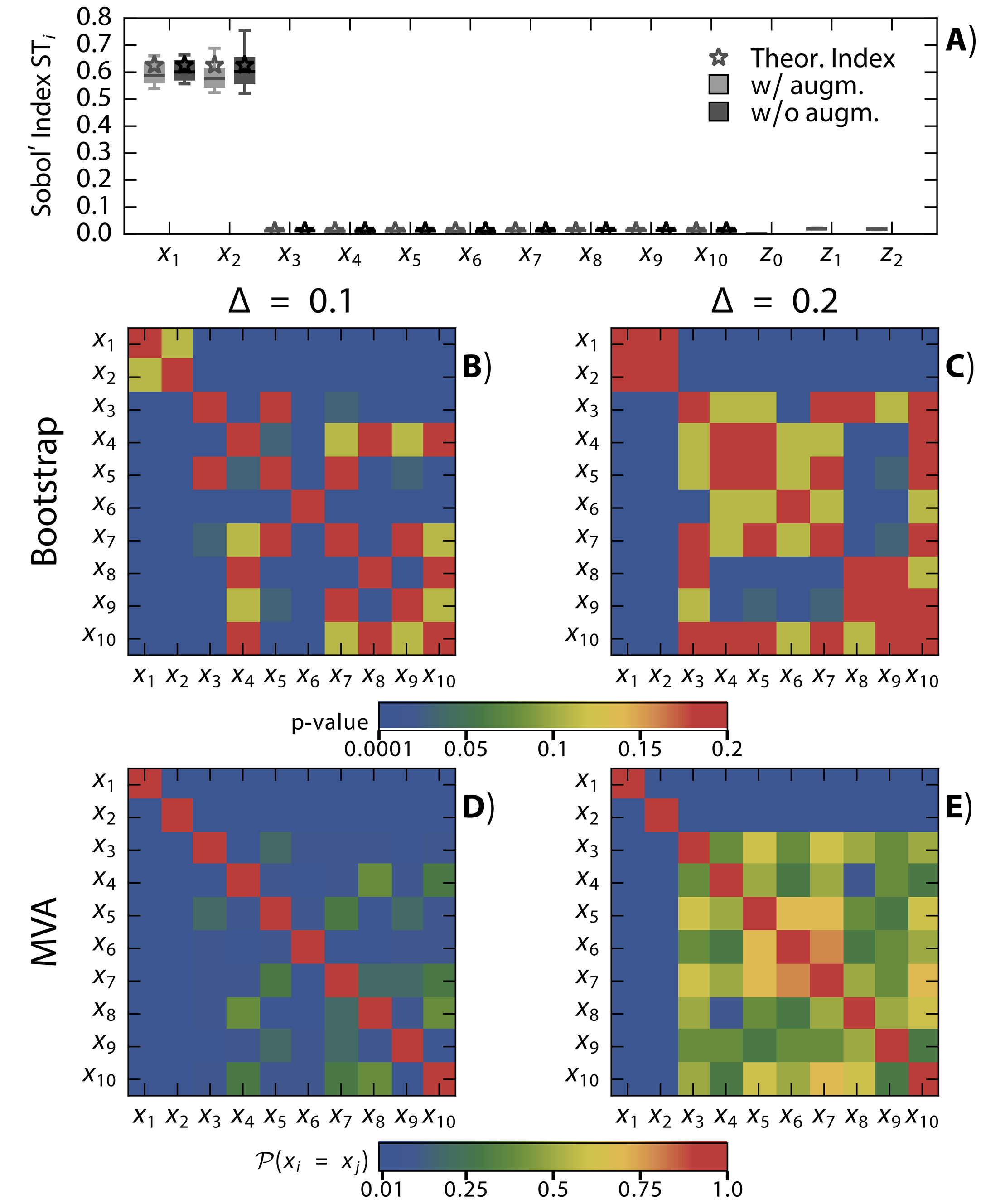


**Fig. 4:** Testing if variables are significantly different. In case of bootstrapping the Kolmogorov-Smirnov test is applied (B, C). Low p-values indicate distinguishable variables. In case of MVA, variables whose difference is smaller than the difference between the augmented variables are identified to be indistinguishable. Plots D and E show the probability that a pair of variables is distinguishable.

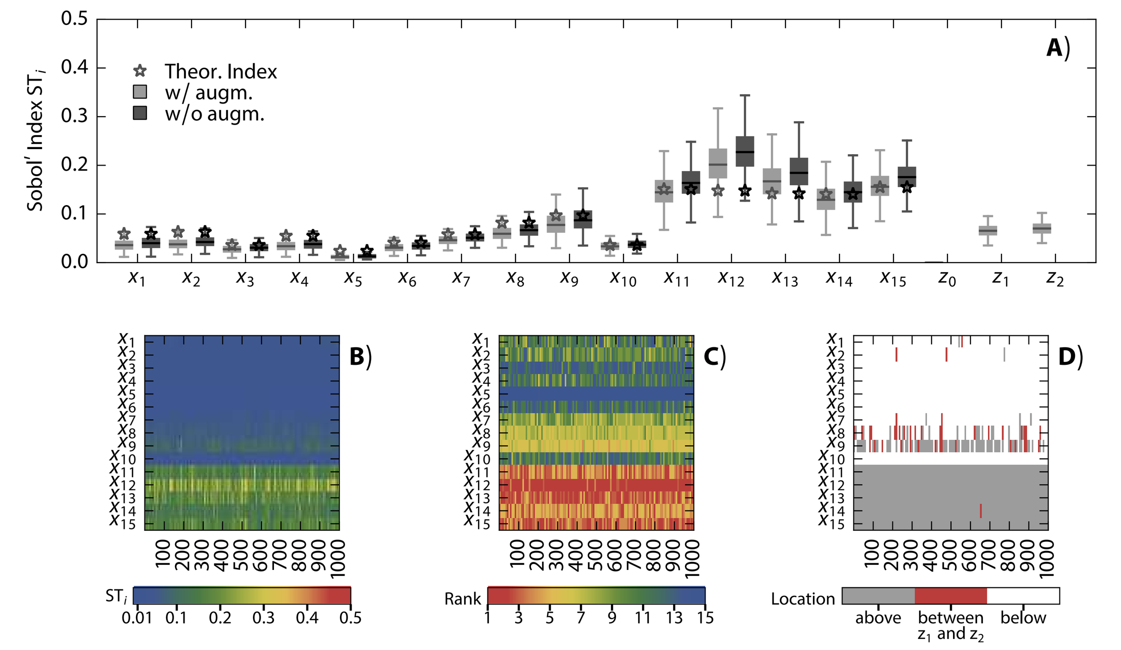


**Fig. 2:** Results of a Sobol' sensitivity analysis for the Oakley-O'Hagan test function using 100 reference variable sets and a confidence threshold $\Delta$ of 0.2. The individual subplots are the same as in Figure 1.

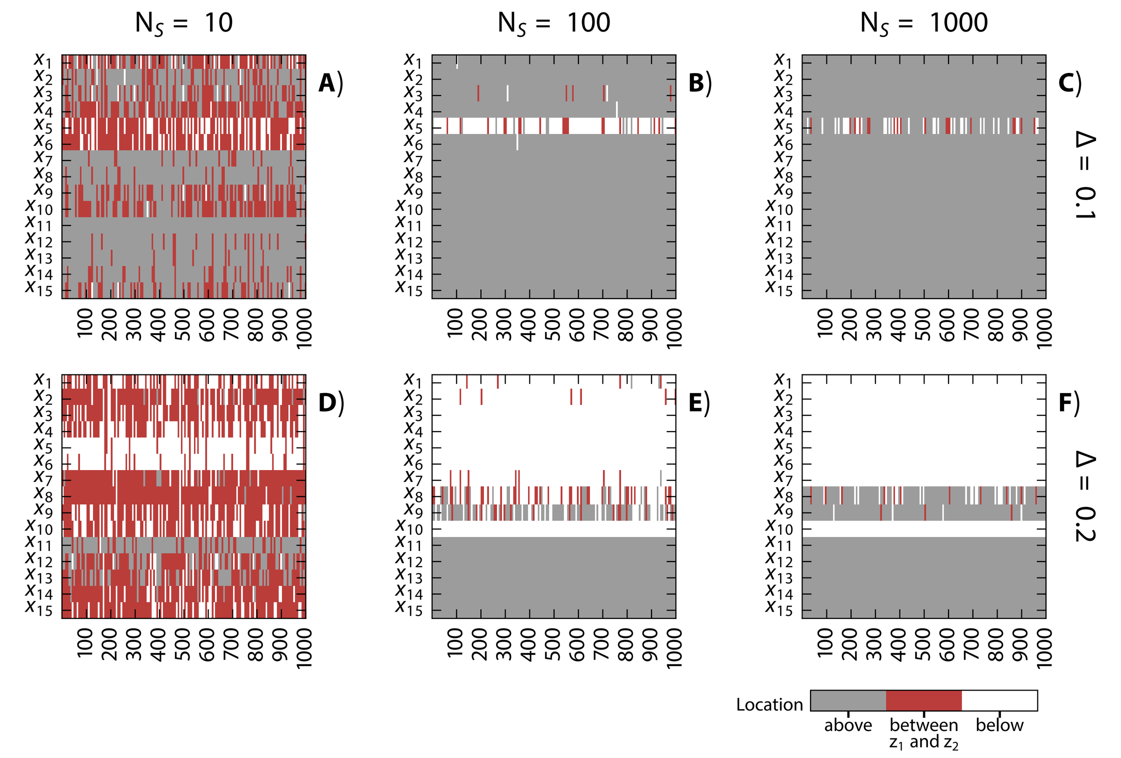


**Fig. 3:** Results of a Sobol' sensitivity analysis for the Oakley-O'Hagan test function using 10, 100, and 1000 reference variable sets ($N_S$) and confidence threshold $\Delta$ of 0.1 and 0.2. The number of variables enveloped by the augmented variables $z_1$ and $z_2$ are a surrogate for non-convergence.

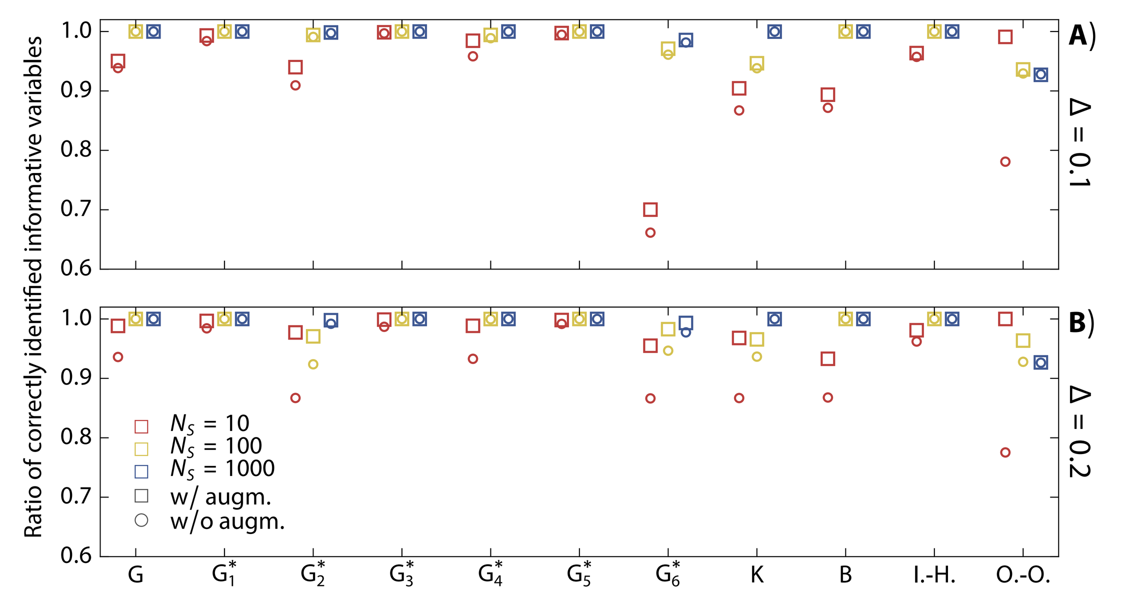


**Fig. 5:** The ratio of correctly determined informative variables using different confidence thresholds $\Delta$ and different numbers of reference sets $N_S$ used to estimate the Sobol' sensitivities. The variable augmentation MVA is increasing the number of correctly identified informative variables in all experiments (compare squares and circles).