What about totals?
Alternative approaches to factor fixing

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ABSTRACT: In global sensitivity analysis, the total effect provides necessary and sufficient information if a model output Y depends on an input factor X. Hence this indicator is of importance if one is trying to identify uninfluential factors in a factor fixing setting. This approach is often used to identify research needs and to focus attention on influential factors.
We remind how suitable sensitivity indicators are obtained and investigate methods of global sensitivity analysis for the factor fixing setting. For this we modify the factor fixing setting: An input parameter is uninfluential if it does not significantly change the conditional output distribution given realisations of this input factors when compared to the unconditional output distribution. Instead of considering the whole output distribution, we may ask for influences in the series of moments. This allows for estimation from given observations.
We discuss the findings on the Level E geosphere transport model.

1 INTRODUCTION

Complex decision making relies upon numerical simulation models. The identification of uninfluential input factors in these simulation models is the purpose of the factor fixing setting in global sensitivity analysis. Here, it is well-known that the total effect provides necessary and sufficient information if a model output Y depends on an input factor X. Hence this indicator is of importance if one is trying to identify uninfluential factors. We remind how the total effect is derived from the functional analysis of variance decomposition. However, the computation of total effects involves the design of a special sample for use with the Sobol' method (Saltelli, Annoni, Azzini, Campolongo, Ratto, and Tarantola 2010). Algorithms for determining total effects directly from a given random sample (i.e. without an intermediate metamodel layer) are currently not available. We therefore have to consider alternative approaches as we want to promote cheap sensitivity analysis methods by reusing existing model input/output observations. The presented approach does not depend on the functional ANOVA decomposition and may therefore be of use in situations where one considers dependent input factors.

2 FUNCTIONAL ANOVA AND SENSITIVITY EFFECTS

We consider a function

$$g: \begin{array}{l} \mathcal{X} \subset \mathbb{R}^k \to \mathcal{Y} \subset \mathbb{R}, \\ (x_1, \dots, , x_k) \mapsto y = g(x_1, \dots, x_k) \end{array} \tag{1}$$

which might be the output of some computer code simulating a complex physical model. In a global sensitivity setting, the inputs become a random vector $\mathbf{X}$ with support $\mathcal{X}$ of known probability law. Then the output is a random variable $Y = g(X)$ with support $\mathcal{Y}$.

Variance-based methods originate from the functional ANOVA decomposition (Hoeffding 1948, Efron and Stein 1981). Following the notation of (Owen 2012), let $\alpha = \{i_1, i_2, \dots, i_r\} \subset \{1, 2, \dots, k\}$ denote any subset of indices, where $|\alpha| = r$ is the cardinality of α. The complementary set is $\sim \alpha = \{1, \dots, k\} \setminus \alpha$. Let $\mathbf{x}_\alpha = (x_{i_1}, x_{i_2}, \dots, x_{i_r})$ be a generic

r-vector with components x_s from $\mathcal{X}_s$ where $s \in \alpha$. Provided that $g(\cdot)$ is square integrable and that the density of $\mathbf{X}$ can be written as product of marginal densities $f_{\mathbf{X}}(\mathbf{x}) = \prod_{i=1}^{k} f_i(x_i)$ the uniqueness of the following representation of $g(\cdot)$ is proven in (Sobol' 1969, Efron and Stein 1981)

$$g(\mathbf{x}) = \sum_{r=0}^{k} \sum_{\alpha:|\alpha|=r} g_\alpha(\mathbf{x}_\alpha) \tag{2}$$

where $\sum_\alpha$ denotes the sum over all subsets of indices of cardinality r and the functions $g_\alpha(\mathbf{x}_\alpha)$ are determined by

$$g_0 = \int_{\mathcal{X}} g(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) \mathrm{d}\mathbf{x}$$

$$g_\alpha(\mathbf{x}_\alpha) = \int_{\mathcal{X}_{\sim\alpha}} (g(\mathbf{x}_\alpha, \mathbf{x}_{\sim\alpha}) - \sum_{\beta \subsetneq \alpha} g_\beta(\mathbf{x}_\beta)) f_{\sim\alpha}(\mathbf{x}_{\sim\alpha}) \mathrm{d}\mathbf{x}_{\sim\alpha} \tag{3}$$

where $\mathcal{X}_\beta = \bigotimes_{j\in\beta} \mathcal{X}_j$ and $f_\beta(\mathbf{x}_\beta) = \prod_{j\in\beta} f_j(x_j)$. Note that g_0 corresponds to the empty index set $\beta = \emptyset$ and is therefore part of the sum in (3). The $g_\alpha(\mathbf{x}_\alpha)$ functions in (3) are orthogonal,

$$\int_{\mathcal{X}} g_\alpha(\mathbf{x}_\alpha) g_\beta(\mathbf{x}_\beta) f_{\mathbf{X}}(\mathbf{x})\, \mathrm{d}\mathbf{x} = 0 \qquad \text{for} \quad \alpha \neq \beta. \tag{4}$$

By orthogonality, the variance $\mathrm{Var}[Y]$ of $Y = g(\mathbf{X})$ then becomes decomposed into

$$\begin{aligned}\mathrm{Var}[Y] &= \int_{\mathcal{X}} (g(\mathbf{x}) - g_0)^2 f_{\mathbf{X}}(\mathbf{x})\, \mathrm{d}\mathbf{x} \\ &= \int_{\mathcal{X}} \left(\sum_{r=1}^{k} \sum_{|\alpha|=r} g_\alpha(\mathbf{x}_\alpha) \right)^2 f_{\mathbf{X}}(\mathbf{x})\, \mathrm{d}\mathbf{x} \qquad (5) \\ &= \sum_{r=1}^{k} \sum_{|\alpha|=r} \mathrm{Var}(\alpha)\end{aligned}$$

where

$$\mathrm{Var}(\alpha) = \int_{\mathcal{X}_\alpha} [g_\alpha(\mathbf{x}_\alpha)]^2 f_\alpha(\mathbf{x}_\alpha)\, \mathrm{d}\mathbf{x}_\alpha. \tag{6}$$

(5) and (6) show that the variance-decomposition of $g(\cdot)$ is in one-to-one correspondence with the underlying function decomposition. The sensitivity effect of an index group α with respect to the interaction of order $|\alpha|$ is then $\frac{1}{\mathrm{Var}[Y]} \mathrm{Var}(\alpha)$. To consider all first and higher-order interactions in the group, we can define a main group effect $S_\alpha = \frac{1}{\mathrm{Var}[Y]} \sum_{\beta\subset\alpha} \mathrm{Var}(\beta)$ and a total group effect $T_\alpha = \frac{1}{\mathrm{Var}[Y]} \sum_{\beta\supset\alpha} \mathrm{Var}(\beta)$. In (Liu and Owen 2006) these indicators are called subset and superset importance. By (2), $1 = S_\alpha + T_{\sim\alpha}$ for all index groups α. Comparing with the variance decomposition formula, we have $S_\alpha = \frac{1}{\mathrm{Var}[Y]} \mathrm{Var}[\mathbb{E}[Y|\mathbf{X}_\alpha]]$ and $T_\alpha = \frac{1}{\mathrm{Var}[Y]} \mathbb{E}[\mathrm{Var}[Y|\mathbf{X}_{\sim\alpha}]]$.

Together with the variance decomposition formula, the following result allows for the computation of these sensitivity indicators.

Proposition 1 ((Sobol' 1993)). *Given an index group α, its group effect satisfies*

$$S_\alpha \cdot \mathrm{Var}[Y] = \mathbb{E}[g(\mathbf{X}_\alpha, \mathbf{X}_{\sim\alpha}) g(\mathbf{X}_\alpha, \mathbf{Z}_{\sim\alpha})] - \mathbb{E}[Y]^2 \tag{7}$$

where $\mathbf{Z}_{\sim\alpha}$ is an independent copy of $\mathbf{X}_{\sim\alpha}$.

For index groups with only one element, we define the first order effect by $S_j = S_{\{j\}}$ and the total effect by $T_j = \sum_{\alpha\ni j} S_\alpha$.

2.1 *The Sobol' method*

The computation of one total effect from the functional ANOVA decomposition derived above involves 2^{k-1} out of 2^k functions, hence it is not effective. A different approach is the Sobol' method (Homma and Saltelli 1996, Saltelli, Annoni, Azzini, Campolongo, Ratto, and Tarantola 2010). It computes first and total effects of factor j by constructing three input samples of realizations $x = (x_1 \ldots x_k)$, $x'_j = (x'_1 \ldots x'_k)$ and $x^*_j = (x^*_1 \ldots x^*_k)$. If $*$ denotes a wild-card then the input realizations associated with x^*_j satisfy the following pattern matching rule $(x_1, \ldots, x_{j-1}, *, x_{j+1} \ldots, x_k)$ compared to the inputs associated with x while those input realizations associated with x' satisfy the rule $(*, \ldots, *, x_j, *, \ldots, *)$. Hence samples for X and X^*_j are drawn from the same distribution conditional to $\mathbf{X}_{\sim j}$ while those for X and X'_j are drawn from the same distribution conditional to X_j.

Theorem 2 (Sobol' duality, (Saltelli, Annoni, Azzini, Campolongo, Ratto, and Tarantola 2010)). *Let X, X'_j and X^*_j be samples of size $n \times k$ constructed as above and set $Y = g(X)$, $Y'_j = g(X'_j)$ and $Y^*_j = g(X^*_j)$. Then the Sobol' estimators for first and total effects are given by the following inner products*

$$\widehat{S}^S_j = \frac{\langle Y'_j, Y - Y^*_j \rangle}{\langle Y - \bar{Y}, Y - \bar{Y} \rangle}, \tag{8}$$

$$\widehat{T}^S_j = 1 - \frac{\langle Y^*_j, Y - Y'_j \rangle}{\langle Y - \bar{Y}, Y - \bar{Y} \rangle}. \tag{9}$$

Alternatively, the Jansen estimators are given by

$$\widehat{S}_j^J = 1 - \frac{1}{2}\frac{\langle Y - Y_j', Y - Y_j'\rangle}{\langle Y - \bar{Y}, Y - \bar{Y}\rangle}, \tag{10}$$

$$\widehat{T}_j^J = \frac{1}{2}\frac{\langle Y - Y_j^*, Y - Y_j^*\rangle}{\langle Y - \bar{Y}, Y - \bar{Y}\rangle}. \tag{11}$$

Here $\bar{Y} = \frac{1}{n}\sum_{i=1}^n y_i$ *is the output sample mean.*

The Jansen estimator for total effets requires only the X and X_j^* samples. Unfortunately, in quasi Monte-Carlo design this "all-fixed-but-one" condition is to be avoided (Sobol' 1979). Hence weakening the condition of exact matches for an estimator from given samples is likely to fail for a quasi Monte-Carlo input design.

Surrogate modelling approaches include the following two ideas: One can construct a k-dimensional metamodel and create Sobol' samples with respect to this meta-model. Alternatively, one may compute the goodness-of-fit for an $k-1$ dimensional model.

3 FACTOR FIXING

We have seen that the computation of total effects is not straight-forward. We therefore have to review the foundations. Hence let us formulate the underlying assumption of the factor fixing model: *An input parameter is deemed to be uninfluential if its direct influence on the output (measured by the first order effect) and its indirect influence via interactions on the output (measured by higher order effects) are negligible.* The sum of first and higher order effects is collected in the total effect which is therefore the indicator of choice in a factor fixing scenario. Hence if Y is not influenced by X_j for all index sets β in the functional ANOVA decompositions the variance contributions containing factor j vanish $\mathrm{Var}(\{j\} \cup \beta) = 0$. The unconditional random variable $Y = Y|(X_j, \mathbf{X}_{\sim j})$ (i.e. Y is a function of X_j and $\mathbf{X}_{\sim j}$) is the same as the conditional random variable $Y|\mathbf{X}_{\sim j}$. But this also implies that conditioning on X_j does not change the distribution of Y. Hence, we want to use the following description as the basis of our factor fixing considerations: *An input parameter is deemed to be uninfluential if it does not significantly change the conditional output distribution given realisations of this input factors when compared to the unconditional output distribution.* A measure which is able to capture this effect is Borgonovo δ (Borgonovo 2007),

$$\delta_j = \frac{1}{2}\int f_j(x)\int \left|f_Y(y) - f_{Y|X_j=x}(y)\right| dy\, dx. \tag{12}$$

For δ there exist estimators (Plischke, Borgonovo, and Smith 2013) which use available observations. One may consider computationally less demanding variants which replace the L^1 norm of the PDFs with Kolmogorov-Smirnov or Kuiper distances of CDFs,

$$\beta_j = \int f_j(x) \sup_y \left|F_Y(y) - F_{Y|X_j=x}(y)\right| dx, \tag{13}$$

$$\kappa_j = \int f_j(x)\big(\sup_y (F_Y(y) - F_{Y|X_j=x}(y)) - \inf_y (F_Y(y) - F_{Y|X=x}(y))\big) dx. \tag{14}$$

Instead of considering the whole output distribution and its conditionals, we may ask for influences in the series of moments. Such an approach has been suggested by (Ratto, Pagano, and Young 2009) for approximating δ. Hence we can consider the first order effects of higher moments of the output,

$$S_j^{(\ell)} = \frac{\mathrm{Var}\left[\mathbb{E}\left[(Y - \mathbb{E}[Y])^\ell \middle| X_j\right]\right]}{\mathrm{Var}\left[(Y - \mathbb{E}[Y])^\ell\right]}, \tag{15}$$

which can be estimated from given data using methods presented in (Plischke 2010, Plischke 2012b). For first order effects there are graphical methods available (Plischke 2012a) which are used for the analysis the following example.

4 EXAMPLES

Let us have a look at the cusunoro curves introduced in (Plischke 2012a) to visually represent the parameter sensitivities. These curves capture the deviation of the output from the mean value by sampling $u \mapsto \mathrm{Var}[Y]^{-\frac{1}{2}}\,\mathbb{E}\left[Y - \mathbb{E}[Y] \,\middle|\, X_i \le F_{X_i}^{-1}(u)\right]$. For the curves associated with second central moments, the sample y is replaced by $(y-\bar{y})^2$. The cusunoro curves of the Ishigami model (Saltelli, Chan, and Scott 2000) are shown in Figure 1. Especially the third parameter which has null first order effect (left graph) shows up at the second central moment (right graph). The fourth parameter which is a dummy stays close to zero hence conditioning on it will neither change the output Y nor of its squared centralized value $(Y - \mathbb{E}[Y])^2$, i.e., there is no functional depencency of X_4 for both the mean and the variance of Y.

All computational methods for computing first order effects can be augmented to take advantage of these higher moment effects by not only considering the model output directly, but also transformations of the model output, i.e. computing $S_j^{(\ell)}(Y) = S_j((Y - \mathbb{E}[Y])^\ell)$.

Let us remind how first order effects are obtained from given observations. From the functional ANOVA decomposition, we have $g_{\{j\}}(x_j) = \mathbb{E}[Y|X_j = x_j] - \mathbb{E}[Y]$, hence knowing the nonparametric regression curve $\varphi_j(x_j) = \mathbb{E}[Y|X_j = x_j]$ for

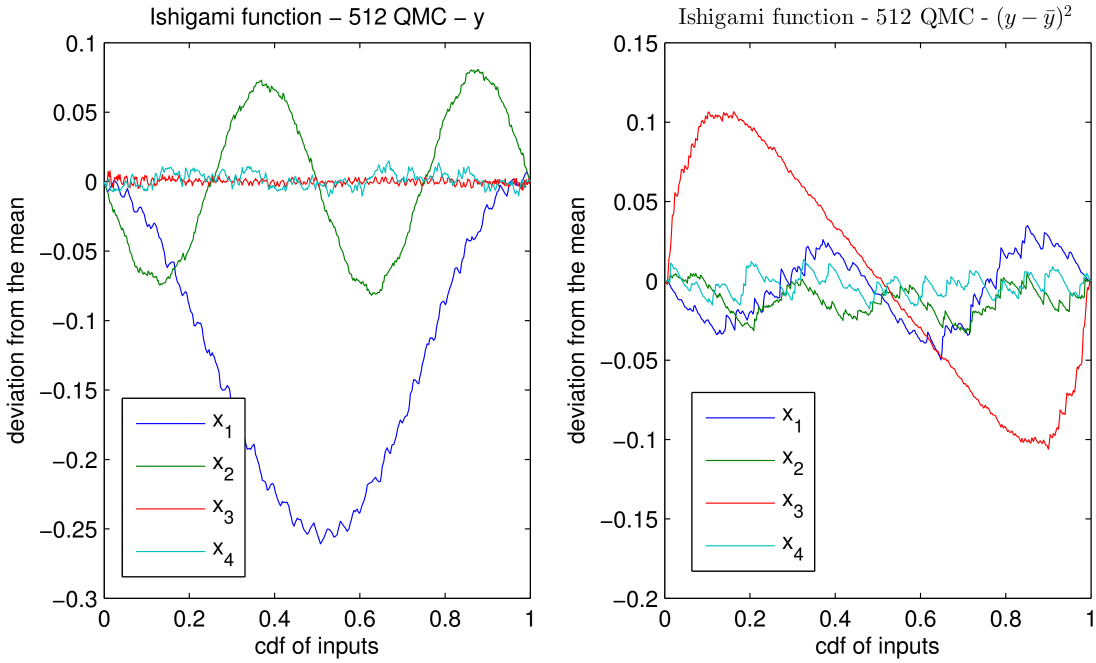

Figure 1: CUSUNORO curves for first and second centralized moments, quasi Monte Carlo sample of size 512.

given realizations leads to the estimator

$$\widehat{S}_j^{\varphi} = \frac{\sum_{i=1}^{n} \left(\varphi(x_{ij}) - \bar{y}\right)^2}{\sum_{i=1}^{n} \left(y_i - \bar{y}\right)^2} \tag{16}$$

which is a nonlinear goodness-of-fit or coefficient of determination (Doksum and Samarov 1995). Given a (finite) orthonormal function system with respect to the inner product $\langle \varphi, \psi \rangle_j = \int_{\mathcal{X}_j} \varphi(x_j)\psi(x_j) f_{X_j}(x_j)\, \mathrm{d}x_j$ for approximating $g_{\{j\}}(\cdot)$ the associated regression coefficients can be used directly without considering the model prediction (as Parseval's Theorem holds for the variance decomposition). This is the basic idea behind polynomial chaos approaches to global sensitivity analysis (Lewandowski, Cooke, and Duintjer Tebbens 2007, Sudret 2008).

Let us consider the effective algorithm for sensitivity indices, using the cosine transformation (COSI) (Plischke 2012b) which works on given observations and the random balance design (RBD) (Plischke, Tarantola, and Mara 2013) which needs a specially constructed sample, but allows for small sample sizes. Furthermore, we consider a δ estimator (Plischke and Borgonovo 2013) and total effects using the Sobol' method utilizing Prop. 1. Table 1 shows some simulation results which fully support our findings from the graphical interpretation. The COSI method is applied to a quasi Monte Carlo sample of size $n = 511$, the RBD method uses also $n = 511$ realizations which are quasi-randomly permuted. The Sobol' method uses a sample size of $n = 511$. The implementation needs two basic samples A and B so that $A_j^* = B_j'$ hence $(k+2) \cdot n$ model evaluations are needed ($k = 4$). Choosing a sample size where a Monte Carlo error of 1% can be expected, the δ estimation uses $n = 2^{14} - 1$ with $M = 63$ partition classes and an empirical cdf-based approach. From this partition, S_j has also been estimated using a correlation ratio estimator (Pearson 1905, Plischke 2012a).

All of the indicators $S_j^{(2)}$, T_j and δ_j show that factor $j = 3$ has a non-null effect on the output, however this is not visible by first order effects where all estimates yield comparable results. The computational cost for arriving at this conclusion varies greatly.

These methods are less suited for producing a ranking list of influential factors, note that total effects ranks factors 1–2–3–4 while δ ranks 2–1–3–4 and considering $\max_\ell S_j^{(\ell)}$ as an indicator, the list reads 2–3–1–4. But they all succeed in identifying the dummy parameter $j = 4$.

One major advantage which has not been mentioned is that for the computation of total effects, independence of the marginal distributions of the input is required. Although there are many efforts to weaken this assumption (Xu and Gertner 2007, Li, Rabitz, Yelvington, Oluwole, Bacon, and Kolb 2010, Mara and Tarantola 2012) there has been no consensus reached about what to do in dependent input scenarios. On the other hand, first order effects of higher moments require just the marginal probability.

4.1 *The Level E geosphere transport model*

In many publications, the PSACOIN Level E code (Nuclear Energy Agency 1989) is used both as a benchmark of Monte Carlo simulations and as a benchmark for sensitivity analysis methods. A review is available in (Saltelli and Tarantola 2002).

Together with the COSI estimator the higher moments first order effects method is able to act as a post-processor so that we can dust off a dataset, a quasi-

Table 1: Numerical experiments, Ishigami function

Factor	COSI				RBD			Sobol'		Delta	
j	S_j	$S_j^{(2)}$	$S_j^{(3)}$	$S_j^{(4)}$	S_j	$S_j^{(2)}$	$S_j^{(3)}$	S_j	T_j	S_j	δ_j
1	0.3151	0.0647	0.1709	0.0484	0.3193	0.0644	0.1773	0.3167	0.5585	0.3111	0.2542
2	0.4434	0.0401	0.1186	0.0177	0.4521	0.0028	0.1474	0.4543	0.4577	0.4389	0.4311
3	0.0001	0.3180	0.0016	0.2342	0.0004	0.3005	0.0014	0.0094	0.2485	-0.0038	0.2092
4	0.0004	0.0172	0.0010	0.0229	0.0009	0.0198	0.0085	0	0	-0.0037	0.0147

Monte Carlo sample of size $n = 8192$ with $k = 12$ parameters and the associated output vector, from the electronic shelf and analyse it.

Density-based sensitivity indicators as presented in (12), (13) and (14) are invariant with respect to monotonic transformation of the output. In order to obtain similiar results using variance-based indicators, we do not analyse the output Y directly, but in form of the empirical CDF, U with $u_{i:n}(y) = \frac{1}{2n}\left(2\#\{y_j < y_i\} + \#\{y_j = y_i\} + 1\right)$.

Figure 2 shows the time dependent sensitivity results using the distribution based sensitivity indicators and the first order effects of higher moments for the empirical output CDF of the total dose. We see that the Smirnov, Kuiper and Borgonovo sensitivity are offering the same information content, however, present a high level of numerical noise. In a factor fixing setting this has to be avoided. Moreover, note that in the lower graphics the third moment plot does not offer additional information compared to the first moment plot.

The parameter v^1 (velocity in geosphere layer 1) is rated important through all of the considered time frame, while the importance of l^1 (length of geospere layer 1) has a local minimum at $t = 10^5$ (due to a switch from the Iodine dominated regime to the Neptunium decay chain). A closer look in the lower plots of Figure 2 shows that the contributions from W (biosphere steam flow rate) and v^2 (velocity in geosphere layer 2) are influencing the second moment, not the first moment. The distribution based indicators may be thought of as an overlay of these higher moment plots. The second-moment importance of W is in contrast to an analysis of the variance based sensitivity of the raw data where it immediately shows up as important in the first moment, however the overall expanatory power of the regression model on the raw data is much smaller, see (Plischke 2010).

4.2 *Conclusions*

This note shows that in a factor fixing setting there are other indicators than total effects available which have a small computational fingerprint and offer additional theoretical advantages.

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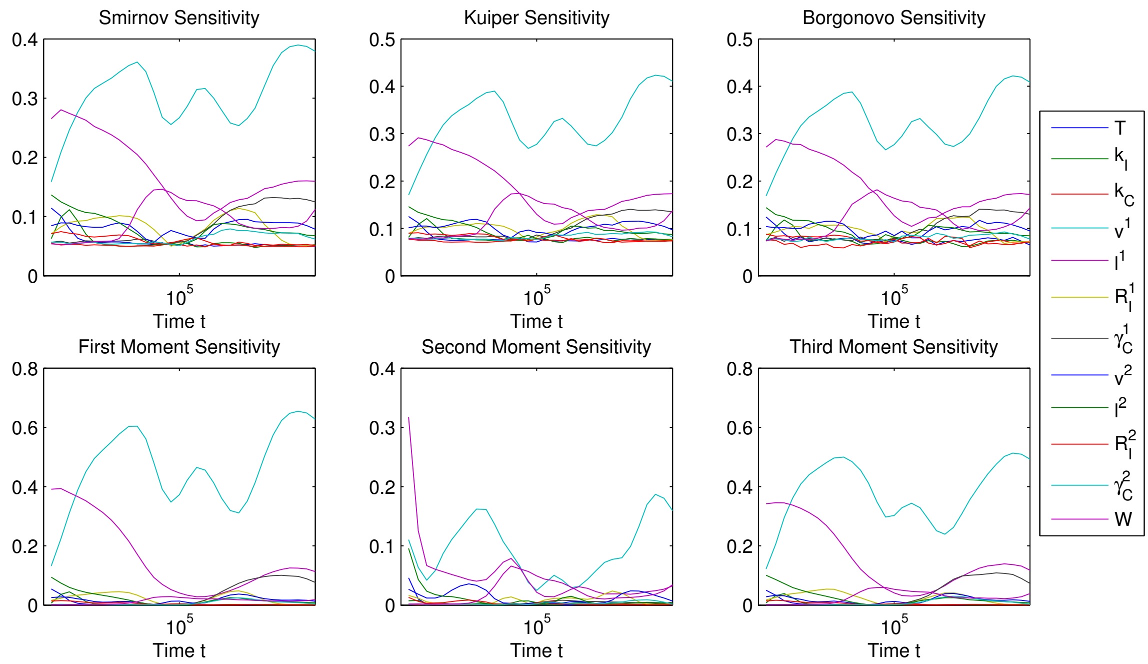

Figure 2: Time-dependent sensitivity indicators for the Level E model, 8192 QMC. Variance-based indicators are computed on ranks.

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