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Speaker: Laura Swiler

Metamodelling sensitivity approaches versus regression and graphical methods on the basis of Geologic Cases: An International Collaboration

Laura Swiler, Dusty Brooks, Emily Stein
Sandia National Laboratories, USA
lpswile@sandia.gov, dbrooks@sandia.gov, ergiamb@sandia.gov
Klaus-Jürgen Röhlig, Elmar Plischke
Institute of Disposal Research, TU Clausthal, Germany
klaus.roehlig@tu-clausthal.de, elmar.plischke@tu-clausthal.de
Dirk-Alexander Becker, Sabine Spiessl
Repository Safety Department, GRS, Germany
Dirk-Alexander.Becker@grs.de, sabine.spiessl@grs.de
Lasse Koskinen, Pekka Kupiainen
Posiva, Finland
Lasse.Koskinen@Posiva.fi, Pekka.Kupiainen@posiva.fi
Joan Govaerts
Belgian nuclear research centre, SCK-CEN, Belgium
joan.govaerts@sckcen.be
Valentina Svitelman, Elena Saveleva
Nuclear Safety Institute of the Russian Academy of Science, Ibrae, Russia
svitelman@ibrae.ac.ru, saveleva@ibrae.ac.ru

Over the past four years, an informal working group has developed to investigate existing sensitivity analysis methods, identify best practices, and examine new sensitivity analysis methods being developed. The focus is on the use of sensitivity analysis in case studies involving geologic disposal of spent nuclear fuel or nuclear waste. We have developed multiple applicable case studies to use for testing ideas and making comparisons.[1] Four of these case studies are discussed: the GRS clay case, the SNL shale case, the Dessel case, and the IBRAE groundwater case. We present the different sensitivity analysis methods investigated by various groups, the results obtained by different groups and different implementations, and summarize our findings.

The case studies focused on repository models for underground disposal of nuclear waste. The four case studies typically included things such as a waste form (canister or steel drum encasing the waste), an engineered buffer such as bentonite or concrete, and modeling of a natural system. The processes modeled in the case studies included waste package degradation, radionuclide dissolution, radionuclide sorption and precipitation/ dissolution, radioactive decay, and radionuclide transport via advection and diffusion. The number of uncertain input parameters ranged from 6 to 20 in these case studies. The outputs included time-series data (e.g. radionuclide concentrations as a function of time and/or spatial location), dose rates, fluxes, etc.

The participating groups used a large variety of sensitivity analysis methods: scatterplots, simple correlation coefficients, rank correlation coefficients, standardized regression coefficients, main and total effects variance-based Sobol' indices estimated by methods such as EASI, RBD-FAST, distribution-based methods such as PAWN, graphical methods like CUSUNORO, and others. For each geologic case study, multiple groups presented their results using different sensitivity analysis methods and/or different implementations of the same method. The breadth and scope of the case studies as well as the number of methods used provided a rich environment to study and compare results.

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We found that the first order variance-based index estimates can be easily generated from observational data (i.e. existing data which were not generated by prescribed sampling schemes) using a variety of approaches and are one of the preferred SA approaches. Linear and rank correlation coefficients and regression approaches continue to be used and are informative. More advanced methods show results mostly consistent with simpler methods but there are important differences. Graphical methods such as CUSUNORO also provide additional visualization which can show influences over the range of a variable.

We found consistency between the linear sensitivity measures (correlation and regression coefficients) calculated by the different partners but sometimes the variance-based sensitivity indices did not rank the important variables in agreement with the linear sensitivity measures. Also, there were more differences in rankings seen across the variance-based sensitivity indices from different methods, such as EASI/RBD-FAST, EFAST, PCE and RS-HDMR. Note that some of the variance-based methods make direct use of the simulation results for calculating the sensitivity indices while other methods use them to train surrogate or metamodel approximations of the simulation. All the methods used in this study relied on fixed data sets generated by the case study owners: specialized sampling of the simulations was not possible.

Parameter rankings obtained by Sobol' method are mostly consistent among different sample sizes and different surrogate models, however, there are often visible numerical issues for small sample sizes such as: negative main indices or conversely main indices slightly higher than total indices for parameters with minor or no significance, or sum of main indices more than one. This can be due to insufficient samples to accurately calculate the integrals defining the terms in the Sobol' index calculations and/or surrogate inaccuracies. We note that the choice of sampling method is of paramount importance to the resulting accuracy of both surrogate models and values of Sobol' indices.

In summary, these four cases provided a realistic set of data to study the differences in sensitivity analysis methods and implementations. We plan to continue this work with even more challenging case studies of geologic repositories, with a focus on time-dependent, highly nonlinear and/or non-monotonic behavior and inclusion of features such as spatial heterogeneity of fracture fields.

[1]: Laura P. Swiler, Dirk-Alexander Becker, Dusty Brooks, Joan Govaerts, Lasse Koskinen, Pekka Kupiainen, Elmar Plischke, Klaus-Jürgen Röhlig, Elena Saveleva, Sabine M. Spiessl, Emily Stein, Valentina Svitelman. "Sensitivity Analysis Comparisons on Geologic Case Studies: An International Collaboration." In preparation.

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