7th International Conference on
Sensitivity Analysis
of Model Output

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University of Nice, Valrose Campus

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Oral presentations
Proceedings

SAMO 2013 - July 1st-4th 2013

University Nice Sophia Antipolis, Valrose Campus, Nice, France

7th International Conference on Sensitivity Analysis of Model Output

Scope of the conference

Modelling activities are steadily increasing in all scientific disciplines, ranging from financial to environmental assessments. Sensitivity Analysis is crucial both in the modelling phase and in the interpretation of model results. It contributes to model development, model calibration, model validation, reliability and robustness analysis, decision-making under uncertainty, quality-assurance, and model reduction.

SAMO conferences are devoted to advances in research on sensitivity analysis methods and their interdisciplinary applications, they are held every third year. The aim of the conference is to bring together researchers involved in the developments and improvements of methods and strategies and users of sensitivity analysis in all disciplines of science, including physics, operations research, chemistry, biology, nanotechnology, engineering, environmental science, nuclear and industrial safety, economics and finance, etc.

The first day (July 1) is organized jointly with the MASCOT-NUM network and is devoted to presentations by PhD students working on the topics covered by the SAMO conference and MASCOT-NUM (uncertainty in simulation, sensitivity analysis, design and modelling of computer experiments, model validation, optimization under uncertainty, applications, etc.). A submission call has been launched to PhD students. Eight PhD students have been selected for oral presentations, other student submissions being considered for poster communications. A prize of 1000€ will be conferred by the MASCOT-NUM's scientific committee to the best student communication (to be used by the student to go to a meeting).

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Plenary lectures

Jacques Blum (University of Nice-Sophia Antipolis, France) - Back and Forth Nudging for data assimilation in geophysics

Dick Den Hertog (Tilburg University, the Netherlands) - Robust optimization using computer experiments

Holger Dette (Bochum University, Germany) - Design for linear models with correlated observations

Silvio Funtowicz (Bergen University, Norway) - Models of science and policy

Fabrice Gamboa (Institut Mathématique de Toulouse, France) - Fast and Sobol Pick Freeze methods in the Costa Brava sauce

Andrea Saltelli (JRC Ispra, Italy), Silvio Funtowicz, Sjoerd Hardeman (Bergen University, Norway), Michaela Saisana (JRC Ispra, Italy) - Sensitivity auditing

Back and Forth Nudging for data assimilation in geophysics

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Data Assimilation is the ensemble of techniques combining in an optimal way (in a sense to be defined) the mathematical information provided by the equations of the model and the physical information given by the observations in order to retrieve the state of a flow [1]. There are two large classes of methods: variational algorithms (4D-VAR) and sequential techniques (Kalman filtering).

The standard nudging algorithm is a simple data assimilation technique: it consists in adding to the state equations of a dynamical system a feedback term, which is proportional to the difference between the observation and its equivalent quantity computed by the resolution of the state equations. The model appears then as a weak constraint, and the nudging term forces the state variables to fit as well as possible to the observations. This is known in control theory as being the Luenberger's observer. First used in meteorology, the nudging method has been applied with success in oceanography.

The back and forth nudging algorithm, introduced in [2], consists in solving first the forward nudging equation and then the direct system backwards in time with a feedback term which is opposite to the one introduced in the forward equation. This term stabilizes this backward resolution, which is usually ill-posed for these irreversible geophysical systems. The "initial" condition of this backward resolution is the final state obtained by the standard nudging method. After resolution of this backward equation, one obtains an estimate of the initial state of the system. These forward and backward resolutions (with the feedback terms) are repeated until convergence of the algorithm.

This algorithm has been tested for various systems in geophysics [3], such as Lorenz system, viscous Burgers equation, quasi-geostrophic model , or shallow water equations [4] and compared with 4D-VAR method. The convergence of this algorithm has been studied for linear transport equations and non-linear Burgers equation, with or without viscosity in [5]. An improvement to the Back and Forth Nudging (BFN) algorithm for handling diffusion in the context of geophysical data assimilation, in which the sign of the diffusion term is changed in the backward integrations, has been introduced in [6] and the convergence of this algorithm has been studied, in particular for linear transport equations. This modified BFN has been applied to Burgers equations and compared with other algorithms [7].

References

[1] J. Blum, F.-X. Le Dimet, I. M. Navon, Data assimilation for geophysical fluids, Handbook of Numerical Analysis, Vol.14, R. Temam and J. Tribbia editors, North-Holland (2009) 385-441.

[2] D. Auroux, J. Blum, Back and forth nudging algorithm for data assimilation problems, C. R. Acad. Sci. Paris, Ser. I 340 (2005) 873–878.

[3] D. Auroux, J. Blum, A nudging-based data assimilation method: the back and forth nudging (BFN) algorithm, Nonlinear Processes in Geophysics 15 (2008) 305-319

[4] D. Auroux, The back and forth nudging algorithm applied o a shallow water model, comparison and hybridization with the 4D-VAR, International Journal for numerical methods in Fluids (2009) 61:911-929

[5] D. Auroux, M. Nodet: The back and forth nudging algorithm for data assimilation problems: theoretical results on transport equations, ESAIM: COCV Volume18- 02 (2012) 318 - 342

[6] D. Auroux, J. Blum, M. Nodet: Diffusive Back and forth nudging (BFN) algorithm, C. R. Acad. Sci. Paris, Ser. I 349 (2011) 849854

[7] D. Auroux, P. Bansart, J. Blum: An evolution of the back and forth nudging for geophysical data assimilation: application to Burgers equation and comparisons, Inverse Problems in Science and Engineering, DOI:10.1080/17415977.2012.712528

7th International Conference on Sensitivity Analysis of Model Output, July 1-4 2013, Nice

Robust optimization using computer experiments

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The goal of many experiments is to estimate the best solution for a given practical problem. Such experiments may be conducted with a physical system (e.g., an airplane model in a wind tunnel) or a mathematical model of a physical system (e.g., a computerized simulation model of an airplane or an inventory management system). These experiments produce data on the outputs and the inputs. Output may be univariate (a single or scalar response) or multivariate (multiple responses). The number of inputs may range from a single input to many inputs. The inputs may be controllable or uncontrollable (also called environmental inputs).

Robust Parameter Design (RPD) developed in statistical quality control use metamodels (such as regression, Kriging, etc.) estimated from experiments with both controllable and environmental inputs. RPD assumes known mean and covariance, and sometimes even a known distribution of the environmental inputs. In practice such a distribution is often not known, and the final solution may be very sensitive to estimates for the mean and covariance.

We describe a new approach for RPD that uses only experimental data, so it does not need such assumptions. This new approach uses techniques from Robust Optimization, which is a relatively new and important field in mathematical optimization. We show that this new method can be used for many classes of metamodels, including polynomials obtained via regression and Kriging models. Moreover, we describe an adjustable RPD approach in which the values of (some of) the controllable factors are adjusted after observing the values of (some of) the environmental inputs. This new method is based on Adjustable Robust Optimization techniques. We illustrate our novel method through several numerical examples, which demonstrate its effectiveness.

This is joint work with Jack P.C. Kleijnen and Ihsan Yanikoglu, both from Tilburg University.

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7th International Conference on Sensitivity Analysis of Model Output, July 1–4 2013, Nice

Design for linear models with correlated observations

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In the common linear regression model the problem of determining optimal designs for least squares estimation is considered in the case where the observations are correlated. A necessary condition for the optimality of a given design is provided, which extends the classical equivalence theory for optimal designs in models with uncorrelated errors to the case of dependent data.

If the regression functions are eigenfunctions of an integral operator defined by the covariance kernel, it is shown that the corresponding measure defines a universally optimal design. For several models universally optimal designs can be identified explicitly. In particular, it is proved that the uniform distribution is universally optimal for a class of trigonometric regression models with a broad class of covariance kernels and that the arcsine distribution is universally optimal for the polynomial regression model with correlation structure defined by the logarithmic potential.

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Models of Science & Policy: From Expert Demonstration to Extended Participation

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Our modern (Western) civilisation is based on science in several ways. Science is the basis of the material culture which has so transformed the world; and it is also a primary source of legitimation for policy arguments. As science-related policy issues have come to be recognised as complex and more inherently difficult of solution, the conception of the role of science has also developed and matured. Today, when science is deployed in the policy context, we are aware of the possibility that facts are uncertain, values in dispute, stakes high and decisions urgent. These last features define what we call a post normal science problem. In the light of this new understanding, we can identify several conceptual models of the relation between science and decision-making in policy processes. We trace their evolution through a deepening appreciation of the process of the use of science in policy.

The 'modern' model (perfection/perfectibility).

Scientific facts (unproblematic), employed in rigorous demonstrations, would determine correct policy. In classical terms, the true entails the good; in modern terms, truth speaks to power. Being based on scientific facts, the power that is exercised is effective. There are no limits to the progress of man's control over his environment, and no limits to the material and moral progress of mankind. This is the classic 'technocratic' vision, dependent on an assumed perfection/perfectibility of science in theory and practice.

Precautionary model (uncertain and inconclusive information).

In real policy processes, it is discovered that the scientific facts are neither fully certain in themselves, nor conclusive for policy. Progress cannot be assumed to be automatic, and control over the environment can fail, leading sometimes to pathological situations. While all sides still pay homage to the truth/validity of science in general, they each contest particular unwelcome items of information. Because of this imperfection in the science, there is an extra, normative, element in policy decisions, precaution, which both protects and legitimises decisions.

Framing (arbitrariness of choice and possible misuse).

In the absence of conclusive facts, scientific information becomes one among many inputs to a policy process, functioning as evidence in the arguments. Debate is known to be necessary, as different stakeholders have their own perspective and values shaping their arguments. Moreover, all such processes involve complex issues, where the situation has a plurality of phases (causes, effects, prevention, remediation, etc.), each with its own theoretical constructions of reality. There are no simple 'facts' that resolve issues in all these phases and aspects. Hence the framing of the relevant scientific problem to be investigated, even the choice of the scientific discipline to which it belongs becomes a prior policy decision, part of the debate among those affected by the relevant issue. Different scientific disciplines become competing stakeholders; whoever 'owns' the research problem will make the greatest contribution and will enjoy the greatest benefits. There is no conclusive scientific basis for the choice of framework, and hence to some extent the choice is arbitrary (or social).

Demarcation (possibility of abuse of science).

The scientific information and advice that are used in the policy process is created by people working in institutions with their own agendas. Experience shows that this context can affect the contents of what is offered, through the selection and shaping of data and conclusions. Although they are expressed in scientific terms, the information and advice cannot be guaranteed to be objective and neutral. In this sense, science can be abused when used as evidence in the policy process. A clear demarcation between the institutions (and individuals) who provide the science, and those where it is used, is advocated as a means of protecting science from the political interference that would threaten its integrity. It also ensures that political accountability rests with policy makers and is not shifted, inappropriately, to the scientists. In addition, it prevents scientists from using the authority of their status as an illegitimate validation of their pronouncements when they engage in partisan advocacy on contentious policy issues. However, too great a separation can result in the scientific institutions pursuing their own, internal goals, and the work becoming irrelevant to the needs of the policy process. Designing the right form of demarcation of science and policy is therefore one of the urgent tasks of governance.

Extended participation

Given these acknowledged imperfections in the deployment of science in the policy process, it becomes ever more difficult to defend a monopoly of accredited expertise for the provision of scientific information and advice. 'Science' (understood as the activity of technical experts) is included as one part of the 'relevant knowledge' is brought in as evidence to a process. The ideal of rigorous scientific demonstration is replaced by that of open public dialogue. Citizens become both critics and creators in the knowledge production process as part of an extended peer community. Their contribution is not to be patronized by such labels as 'local', 'practical', 'ethical' or 'spiritual' knowledge. A plurality of co-ordinated legitimate perspectives (with their own value-commitments and framings) is accepted. The strength and relevance of scientific evidence is capable of assessment by citizens. All sides come to the dialogue ready to learn, or else the process is a sham. Through this co-production of knowledge, the extended peer community creates a democracy of expertise in the context of post normal science.

Summary

We can see the latter four models as a progression from the initial 'modern' model with its assumption of perfection of science in the policy process. All this had initial expressions in the debates of the 1970s, when ‘progress’ started to come into question. It has emerged in the policy domain notably in the last decade, starting with the proclamation of 'precaution' at Rio 1992. The post-normal science framework, a part of this evolution, was already published at the beginning of the 1990s, the decade of ‘sustainability’ and precaution; but it has come to prominence only more recently as a result of the debate on governance. The three models of imperfections can be seen to form a sequence of increasing severity, admitting incompleteness, misuse and abuse. Each is designed to resolve a particular type of anomaly, and in any real situation they may be complementary or in conflict. But in each case, the desire is that the link between science and policy remain direct and unmediated. In the successive models, we see that (a) policy is modified by precaution, (b) problems are framed by stakeholders, or (c) scientists are protected from political interference. But the core activity of the modern model, the experts' (desire for) truth speaking to the politicians' (need for) power, is unchanged. The final model, of extended participation, involves a change in the form of governance. Implementing this is a great challenge of our time; for without it, 'the consent of the governed' in science related policy issues will not be maintained.

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7th International Conference on Sensitivity Analysis of Model Output, July 1-4 2013, Nice

Fast and Sobol Pick Freeze methods in the Costa Brava sauce

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In this talk, we will discuss some recent theoretical advances on sensitivity analysis obtained by researchers of the COSTA BRAVA project [1]. More precisely, we will focus on the following topics:

1. Asymptotic properties of Sobol pick freeze method,

2. A new look of the FAST method,

3. Hoeffding Sobol decomposition for systems with non independent inputs.

References :

[1] Web page of the COSTA BRAVA project, www.math.univ-toulouse.fr/COSTA_BRAVA

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7th International Conference on Sensitivity Analysis of Model Output, July 1-4 2013, Nice

Sensitivity Auditing

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The Joint Research Centre of the European Commission is routinely called to provide input to impact assessment activities involving different services of the Commission. Among the tools deployed in this activity JRC has developed an extension of sensitivity analysis termed sensitivity auditing [Saltelli et al., 2013]. This is an attempt to collect best practices from very different corners about how to ensure quality in models when these are used to the science-policy interface. The use of mathematical models in contested issues has been the subject of intense debate and deliberation [Pilkey and Pilkey, 2007], especially in relation to the issue of model plausibility. Ideally sensitivity auditing is to a model's plausibility – a concept explored in anticipatory science [http://www.cspo.org/projects/plausibility/] - what sensitivity analysis is to a model's appropriateness. In other words while a well-run sensitivity analysis is part of the due diligence expected from a model based analysis, sensitivity auditing tests whether the model can 'stand in court'. Sensitivity analysis, as mandated by existing guidelines as a good practice to use in conjunction to mathematical modeling, is as such insufficient to ensure quality in the treatment of uncertainty of science for policy. When stakes are high, uncertainty is inflated and deflated by opposing parties according to convenience. Policy-related science calls for an extension of the traditional internal, peer review-based methods of quality assurance to higher levels of supervision, where extended participation and explicit value judgments are necessary. By the same token sensitivity analysis must extend beyond the technical exploration of the space of uncertain assumptions when the inference being sought via mathematical modeling is subject to relevant uncertainties and stakes. Sensitivity auditing borrows ideas and strategies from sensitivity analysis (Saltelli et al., 2000, 2010), from the NUSAP system for multidimensional uncertainty assessment (Funtowicz and Ravetz, 1990; Van der Sluijs et al., 2005) and from post-normal science (Funtowicz and Ravetz, 1993). In sensitivity auditing 'what to look for' is as important as 'how to look for' and 'who should do the looking'. We thus provide sensitivity auditing's seven rules to extend sensitivity analysis into sensitivity auditing:

1. Check against rhetoric use of mathematical modeling [is the model being used to elucidate or to obfuscate?];
2. Adopt an 'assumption hunting' attitude [what was 'assumed out'? What are the tacit, pre-analytic, possibly normative assumptions underlying the analysis?];

3. Detect Garbage In Garbage Out (GIGO) [=artificial deflation of uncertainty operated in order to achieve a desired inference at a desired level of confidence];

4. Find sensitive assumptions before these finds you [do not publish your inferences without having mapped the assumptions they rely on, lest someone else does it for you];

5. Aim for transparency [stakeholders should be able to make sense of, and possibly replicate, the results of the analysis];

6. Do the right sums [as more important than 'Do the sums right'; is the viewpoint of a relevant stakeholder being neglected?];

7. Focus the analysis on the key question answered by the model, exploring holistically the entire space of the assumptions [Don't do perfunctory analyses changing one factor at a time].

Of the seven rules listed above only the seventh may be considered as 'technical'; all others imply a call for normative vigilance which can only be implemented by in an appropriate institutional and political framework. We quote relevant regulatory literature and offer a set of present-day examples, from academy, blogosphere, the literate press and society, to argument our rules. It applied to mathematical modeling as well as to statistical indicators of various complexities [Paruolo et al., 2012]. Finally we shall submit sensitivity analysis to a criticism, to investigate if and how sensitivity analysis can promote rather than deter the use of a more reflexive use to mathematical modeling from the community of practitioners. Sensitivity auditing is a new concept, and is part of the training offered by JRC in the context of impact assessment, see http://ipsc.jrc.ec.europa.eu/fileadmin/repository/eas/sensitivity/presentations/Sensitivity_Auditing_22Feb2013.pdf.

References

- Funtowicz, S., and Ravetz., J. 1990. Uncertainty and Quality in Science for Policy. The Netherlands, Kluwer Academic Publishers.
- Funtowicz, S.O. , Ravetz, J.R., 1993, Science for the post-normal age, Futures, **25**(7), 739–755.
- Paruolo, P., Saisana, M., and Saltelli, A., 2012, Ratings and rankings: Voodoo or Science? Journal Royal Statistical Society A, **176** (2), 1-26.
- Pilkey, O.H., Pilkey-Jarvis, L., 2007. Useless Arithmetic. Why Environmental Scientists Can't Predict the Future. Columbia University Press, New York.
- Saltelli, A. , Tarantola, S., and Campolongo, F., 2000, Sensitivity analysis as an
- ingredient of modeling. Statistical Science, **15**(4):377-395.
- Saltelli, A., M. Ratto, S. Tarantola and F. Campolongo, 2012 (Perennial Review of the 2005 paper), Sensitivity Analysis for Chemical Models, Chemical Reviews, **112** (5), pp PR1–PR21, DOI: 10.1021/cr200301u, Publication Date (Web): April 19, 2012.
- Saltelli, A., van der Sluijs, J., Guimarães Pereira, Â., 2013, Funtowiz, S.O., What do I make of your Latinorum? Sensitivity auditing of mathematical modelling, Submitted to Foresight and Innovation Policy, special issue on plausibility, arXiv:1211.2668 [physics.soc-ph]
- Van der Sluijs, J.P., Craye, M., Funtowicz, S., Kloprogge, P, Ravetz, J. and Risbey, J. (2005) 'Combining Quantitative and Qualitative Measures of Uncertainty in Model based Environmental Assessment: the NUSAP System', Risk Analysis, **25**(2), 481-492.

Oral presentations

Floriane Anstett-Collin (Univ Lorraine, France), Thierry A. Mara (Univ.La Réunion, France), L. Denis-Vidal (UTC, France), Jeanne Goffart (University of Savoy, France), UASA of complex models: Coping with dynamic and static inputs

Ignacio Arevalo Martin, Ricardo Bolado-Lavin (JRC Petten, The Netherlands), V. Kopustinskas (JRC Ispra, Italy), Identification of bottlenecks in the EU gas transmission network via Sensitivity analysis

William E. Becker and Andrea Saltelli (JRC Ispra, Italy), Paolo Paruolo (University of Insubria, Italy), Econometric model selection using sensitivity analysis

Emanuele Borgonovo (Bocconi University, Italy), Stefano Tarantola (JRC Ispra, Italy), Elmar Plischke (Clausthal University of Technology, Germany), Max D. Morris (Iowa State University, USA), Transformations and Invariance in Global Sensitivity Analysis

Yann Caniou (Phimeca, France), Bruno Sudret (ETH Zürich, Switzerland), Covariance-based sensitivity indices based on polynomial chaos functional decomposition

Biagio Ciuffo, Vincenzo Punzo, Stefano Tarantola (JRC Ispra, Italy), Marcello Montanino (Univ. Napoli, Italy), Assessing the robustness of sensitivity analysis results. Application to traffic simulation models

Nicolas Durrande (University of Sheffield, UK), David Ginsbourger (University of Bern, Switzerland), Olivier Roustant (Ecole des Mines de St- Etienne, France), A class of ANOVA kernels dedicated to sensitivity analysis

Wouter N. Edeling & Paola Cinnella (Arts et Metiers ParisTech, France), Richard P. Dwight & Hester Bijl (Delft University of Technology, The Netherlands), Bayesian estimates of the parameter variability in turbulence models for the RANS equations

Robert Faivre, Victor Picheny, Herve Monod (INRA, France), Simple and efficient tools to explore complex models in agroecology with an eye on interactions

Jean-Marc Fedou, Gilles Menez, Luc Pronzato, Maria-João Rendas (Univ. Nice, France), Revisiting Morris Method: a polynomial algebra for design definition with increased efficiency and observability

Jean-Claude Fort (Univ. Paris Descartes, France), Thierry Klein, Agnes Lagnoux, Beatrice Laurent (IMT, France), Estimation of the Sobol indices in a linear functional multidimensional model

Anaïs Guaus (INRA France), Aline Bsaibes, Thomas Cartailler (ITK, France), Clementine Prieur (Grenoble University, France), Eric Lebon, Frederic Gerard (INRA, France), Time-dependent sensitivity and uncertainty analyses of an agroclimatic model for the water status management of vineyard

Alexandre Janon (Univ. Lyon 1, France), Maëlle Nodet, Clémentine Prieur (Univ. Grenoble, France), Goal-oriented error estimation for reduced basis method. Application to certified sensitivity analysis

Sergei Kucherenko, B. Delpuech (Imperial College London, UK), Bertrand Iooss (EDF, France), Stefano Tarantola (JRC Ispra, Italy), Application of the control variate technique to the estimation of the total sensitivity indices

Matieyendou Lamboni (JRC Ispra, Italy), New way of estimating Total Sensitivity Indices

Sidonie Lefebvre (ONERA, France), Jean-Pierre Gauchi (INRA, France), Multidimensional Global Sensitivity Analysis for Aircraft Infrared Signature Models with Dependent Inputs

Loic Le Gratiet, Claire Cannamela (CEA, France) & Bertrand Iooss (EDF, France), Multi-fidelity sensitivity analysis

Nicolas Lenz (Univ. Bern, Switzerland), A new class of covariance kernels accounting for non-additivity in high-dimensional Kriging

Olivier Martin, Claude Bruchou, Loic Pages (INRA, France), Usefullness of Sensitivity Analysis for Approximate Bayesian Computation

Xavier Merle, P. Cinnella (Arts et Métiers ParisTech, France), Bayesian quantification of thermodynamic uncertainties in dense gas flows

Werner G. Müller, Helmut Waldl (Univ. Linz, Austria), Luc Pronzato, Joao Rendas (Univ. Nice, France), Efficient Prediction Designs for Random Fields

Miguel Munoz-Zuniga (IRSN), Serguei Kucherenko (Imperial College London, UK), Low cost bounds and estimates of total sensitivity indices based on metamodels

Jiri Nossent, Olkeba Tolessa Leta, Willy Bauwens (Univ. Brussels, Belgium), Assessing the convergence of a Morris-like screening method for a complex environmental model

Paolo Paruolo (Univ. of Insubria, Italy), Michaela Saisana, Andrea Saltelli (JRC Ispra, Italy), Fallacies of rankings and ratings

Elmar Plischke (Clausthal-Zellerfeld Univ., Germany), Stefano Tarantola (JRC Ispra, Italy), Thierry A. Mara (Univ. La Reunion, France), Hiking to Mount Toblerone: Advanced Methods for Random Balance Design

Clementine Prieur, Jean-Yves Tissot (Univ. Grenoble), Estimating Sobol' indices combining Monte Carlo estimators and Latin Hypercube Sampling

Nabil Rachdi (EADS, France), Jean-Claude Fort (Universite Paris Descartes, France), Thierry Klein (IMT, France), Fabien Mangeant (EADS, France), New Sensitivity Indices Subordinated to a Contrast

Olivier Roustant (Ecole Nationale Superieure des Mines de St-Etienne, France), Bertrand Iooss (EDF, France), Jana Fruth, Sonja Kuhnt (TU Dortmund University, Germany), Derivative-based global sensitivity measures for interactions

Nathalie Saint-Geours (Irstea, France), Stefano Tarantola (JRC, France), Vytis Kopustinkas (JRC Ispra, Italy), Ricardo Bolado-Lavin (JRC Petten, the Netherlands), Estimating sensitivity indices using contribution to the sample mean

Sabine S. Spiessl, Dirk-A. Becker (GRS, Germany), Sensitivity Analysis of Final Repository Models Using Quasi-Random Sampling and a Metamodel Approach

Bruno Sudret & Chu V. Mai (ETH Zurich), Derivative-based sensitivity indices based on polynomial chaos expansions

Anke Weber, Andrea Saltelli and William Becker (JRC Ispra), A sensitivity analysis of the birth cohort model for tertiary education attainment 2011-2020

Rastko Živanović (Univ. Adelaide, Australia), Global Sensitivity Analysis for Interpretation of Black Box Functions

7th International Conference on Sensitivity Analysis of Model Output, July 1–4 2013, Nice

UASA of complex models: Coping with dynamic and static inputs

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In many fields, complex systems are modelled by a set of partial differential equations with initial and boundary conditions. For instance, in mechanics or thermodynamics, the PDEs are based on conservation laws. A particular problem is defined by a set of inputs that characterized the system of interest, embedding the initial and boundary conditions. Then, numerical methods are employed to solve the problem. In practice, the system is not accurately defined due to the uncertainty about some inputs. Uncertainty and sensitivity analyses (UASA) can help assess the impact of this lack of knowledge onto the model responses ([1,2]). Let $\boldsymbol{y} = g(\boldsymbol{\omega^d}(x,\theta), \boldsymbol{\omega^s}(\theta), x)$ be the response of interest where: $x \in \mathcal{D}$ is the spatial/time variable, $\boldsymbol{\omega^d}$ is a set of random fields (dynamic inputs) and $\boldsymbol{\omega^s}$ is a set of random variables (static inputs) (see figure 1). As an example, in building energy modelling, $\boldsymbol{\omega^s}$ embeds the thermophysical properties of the materials used in the building while $\boldsymbol{\omega^d}$ represents the weather data.
In this communication, we address the issue of performing UASA with these two kinds of uncertain inputs. Indeed, in the literature, such an issue is rarely addressed (except, for instance, in [3]).

For the sake of simplicity, we assume that random variables are independent and defined by their marginal distribution. The random fields are also assumed independent and normally distributed with mean $\bar{\omega}_i(x)$ and covariance function $C_i(x_1, x_2)$, $i = 1, \cdots, N_d$, N_d denoting the number of dynamic inputs. Monte Carlo based methods can be used to perform UASA of such a model. But, while generating static inputs samples is not an issue, it is not straightforward to generate samples that satisfy the desired random fields distribution. One possibility is to resort to the truncated Karhunen-Loeve (KL) expansion. The former expands a random field as follows:

$$\omega_i^d(x,\theta) \simeq \bar{\omega}_i^d(x) + \sum_{k=1}^{M_i} \sqrt{\lambda_{ki}}\xi_{ki}(\theta) f_{ki}(\theta), \tag{1}$$

where λ_{ki} and f_{ki} are the deterministic eigenvalues and eigenfunctions of the covariance function $C_i(x_1, x_2)$, $\boldsymbol{\xi_i}(\theta)$ is a set of independent standard normal variables and M_i is the number of KL-terms. The eigenmodes depend on the choice of the covariance function and are determined by solving the Fredholm integral equation of the second kind given by:

$$\int_{\mathcal{D}} C_i(x_1, x_2) f_{ki}(x_1) dx_1 = \lambda_{ki} f_{ki}(x_2). \tag{2}$$

Equation (2) can be solved using a wavelet-Galerkin scheme ([4]). The advantage of this approach is to avoid tedious quadratures by using wavelet transform, alleviating computational effort.
In practice, we retain the first M_i eigenmodes that contain the 95% of the variance of the input ω_i^d. The number of eigenmodes retained depends on the choice of the covariance function and may be very different from one input to another. Note that once the eigenmodes are obtained for all the dynamic inputs, UASA of the model output are performed through the random vectors $\{\underbrace{\boldsymbol{\xi_1}, \cdots, \boldsymbol{\xi_{N_d}}}_{\boldsymbol{\omega^d}}, \boldsymbol{\omega^s}\}$. Consequently, the effect of the group of factors $\boldsymbol{\xi_i}$ is the one of the dynamic input ω_i^d. This effect can be estimated with sampling-based methods such as Sobol' method ([5]).

The approach is applied to a building energy model. This model presents dynamic inputs as dry bulb temperature, direct and diffuse radiations, humidity, speed and direction of wind, and static inputs as the thermal properties of the materials. The model response of interest is the energy consumption (scalar output).

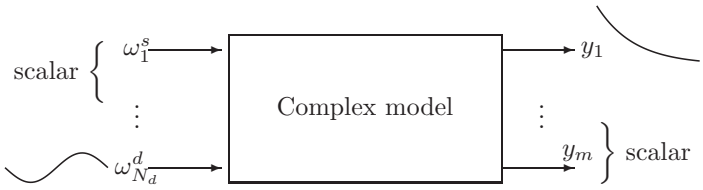

Fig. 1 - Complex model with static and dynamic inputs

References:

[1] A. Saltelli and K. Chan and E. M. Scott, "Sensitivity analysis", *Wiley*, 2000.

[2] E. De Rocquigny and N. Devictor and S. Tarantola, "Uncertainty in industrial practice", *Wiley*, 2008.

[3] L. Lilburne and S. Tarantola , "Sensitivity analysis of spatial models", *International Journal of Geographical Information Science*, **23**:151–168, 2009.

[4] K. K. Phoon and S. P. Huang, "Implementation of Karhunen-Loeve expansion for simulation using a Wavelet-Galerkin scheme", *Probabilistic Engineering Mechanics*, **17**:293–303, 2002.

[5] I. M. Sobol' , "Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates", *Mathematics and Computers in Simulation*, **55**:271–280, 2001.

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Identification of bottlenecks in the EU gas transmission network via Sensitivity Analysis.

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Abstract:

The Russia-Ukraine gas dispute during the winter 2008 / 2009 triggered the hardest gas supply crisis in the EU in the last decade, producing a significant decrease in the amount of gas delivered to customers and important economic losses in eastern European countries. This crisis was the origin of a number of regulatory steps taken by the EU to avoid this type of situation in the future, among them most remarkably the European Energy Programme for Recovery and Regulation 994/2010 on security of gas supply.

One major threat to the security of supply in case of gas crises is the existence of internal bottlenecks in the EU gas transmission network, most remarkably at cross-border points. Broadly speaking, a bottleneck is a network component whose capacity (maximum gas flow allowed by the component in a given direction) is a real obstacle to the transmission of gas in the network, especially in case of crisis (any type of situation that produces some shortage of gas in all or a part of the network). The identification of such bottlenecks, and the development of new infrastructures to remove them, is an important task to increase the resilience and reduce the risk of the EU gas system.

The computer code GEMFLOW, Szikszai and Monforti (2011), was designed at JRC-IET with the intention of investigating the potential effect of gas supply crises with different possible origins (geopolitical crises, technical failure, natural hazards, etc.), and the effect of different measures deployed to mitigate their consequences. This program has been recently modified in order to improve its runtime, incorporate other strategies to cope with gas crises and improve its capabilities to perform Uncertainty and Sensitivity Analysis (UA & SA) using a Monte Carlo approach.

It is important to take into account that the concept of bottleneck, with the purely physical interpretation considered in this work, is very much related to crisis situations. Many bottlenecks arise as a consequence of putting the gas system under big stress, not being detectable in normal situations that do not demand large gas flows. In situation of crisis (for example complete lack of Russian gas coming across Ukraine during a winter cold period with huge gas demand), a clear target of gas system managers is satisfying the demand for as long as possible. In this work we call the number of days during which the demand is satisfied in all Member States (MS) ‘survival time’ of the system.

In order to solve this problem, we develop a strategy based on Monte Carlo filtering (Smirnov two-sample tests) and graphic techniques. The strategy consists in considering the capacity of each pipeline at MS cross-border points an uncertain quantity that follows a uniform distribution between nowadays pipeline capacity and a hypothetical maximum pipeline capacity (the maximum capacity in the EU gas system – the pipeline connecting Ukraine and Slovakia ~ 300 million cubic meters per day – 300

mcm/d) and to run the model under severe crises conditions a number of times (~ 1000), applying the mentioned SA techniques to the results.

Figure 1 shows the type of graphic results obtained. It represents the survival time of the EU gas system (number of days that all EU MS are able to satisfy the demand of gas at peak consumption) for different sampled values of the capacity of the pipeline that connects France with Spain (in this direction, from France to Spain). The results represented have been obtained under the conditions of a huge gas crisis in the Mediterranean Sea where no gas arrives at EU Mediterranean coasts by any means (neither via pipeline nor via Liquefied Natural Gas cargo). GEMFLOW has been run 10,000 times. This figure shows how increasing moderately the capacity (from its nowadays value ~ 8 mcm/d) in the mentioned pipeline does not help increasing the system survival time; only when the capacity exceeds the value 34 mcm/d the system survival time dramatically increases. Equally, increasing it beyond approx. 36 mcm/d does not produce any additional benefit. The statistical significance of these results is supported by the Smirnov two-sample statistical test.

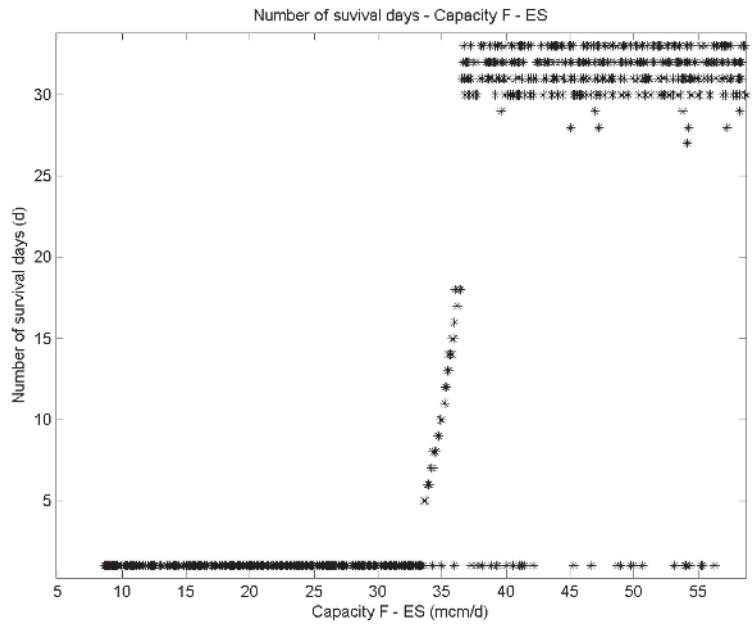

Fig. 1.- Survival days of the EU gas system versus capacity of the pipeline taking gas from France to Spain.

References :

[1] A. Szikszai and F. Monforti, "GEMFLOW: A time dependent model to assess responses to natural gas supply crises", Energy Policy, 39; 5129-5136, 2011.

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Econometric model selection using sensitivity analysis

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A frequent problem of interest to econometricians is that of model selection. Typically a set of time-dependent economic data is available, and it is suspected that some quantity of interest is a function of some unknown subset of these variables. The model selection problem seeks to identify which variables are driving the response, given the data set, and then use these for subsequent forecasts. The problem is typically compounded by lags and strong correlations between the observed data. Standard approaches to this problem are to fit linear models and order variables using t-statistics, then use the F-test to systematically remove spurious regressors until the important variables are found. An influential paper was published which examines and critiques this approach [1], which is the starting point of this work.

The work here proposes a novel application of global sensitivity analysis to deal with econometric model selection. The concept is to assess the sensitivity of some measure of model fit or "quality" to the presence or absence of each variable in the regression model. To give a little more detail, the standard assumption is adopted that the output y is a linear function of a set of D observed variables, $\mathbf{x} = \{x_i\}_{i=1}^{D}$. For any subset of $\mathbf{x}$, a simple linear regression can be fitted with a least squares estimator. There is therefore a set of 2^D possible regression models, representing all possible subsets of regressors, where the choice of regressors in each model k is represented by $\mathbf{z}_k = \{z_{k,i}\}_{i=1}^{D}$, such that $z_{k,i} \in \{0, 1\}$ and $z_{k,i} = 1$ represents the inclusion of x_i in model k and $z_{k,i} = 0$ excludes it. Note that since the estimation of regression parameters is always done by the ordinary least squares approach, each model is completely defined by $\mathbf{z}$. Now, defining η as a function that gives a measure of "model quality" (here the Bayesian Information Criterion is used), the model quality q of a given model can be defined as $q = \eta(\mathbf{z})$. The proposal of this article is to perform a sensitivity analysis on this function η: examining the sensitivity of q to the choices of regressors $\mathbf{z}$. By treating $\mathbf{z}$ as a random binary vector, the total sensitivity index S_T can be calculated for each variable, giving a measure of the contribution to the model quality, and thereby providing a way to distinguish influential variables from non-influential ones.

Using this paradigm, an algorithm was constructed which calculates S_T for each z_i and ranks variables in order of importance. This ranking enables a reasoned search process, whereby candidate regression models are built starting with the regressor with highest S_T, then successively adding regressors in order of importance and using the F-test as a stopping criterion.

In order to test the new approach, the new algorithm, as well as that created in [1], were applied to the same 11 data generating processes (DGPs) used in that study, to see how often the true regressors are recovered. By comparing both optimum performance (by optimising tuning parameters in both algorithms), and performance when tuning parameter values are not known, it was found that the new algorithm outperforms that of [1], such that the rate of not recovering the true DGP was roughly halved. Additionally the new algorithm appears to be significantly more robust.

References:

[1] K.D. Hoover and S.J. Perez, "Data mining reconsidered: encompassing and the general-to-specific approach to specification search", *Econometrics Journal*, **2**:167–191, 1999.

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Transformations and Invariance in Global Sensitivity Analysis

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Modern scientific codes capture a variety of phenomena, from social to physical laws, especially in the environmental and climate change sciences. This generates two types of issues in sensitivity analysis. The first is computational burden (*the curse of dimensionality*, [6]). The statistics literature has addressed this problem extensively since the mid '90's [8, 4] and a series of seminal works on the subject has shown the possibility of abating computational burden drastically, opening the door for application of global methods even to computationally intensive models. This evolution, however, leads to the second problem, namely estimation accuracy, which is the subject of investigation of this work. In several applications, the output of numerical codes is severely skewed and ranges over several order of magnitudes. A commonly-used solution is to transform the output to a logarithmic scale, leading to much more accurate estimation at reasonable sample sizes. But while the estimation quality improves, the global sensitivity statistics lose their original meaning relative to the input-output mapping. We argue that a practical way to avoid this problem is to use global sensitivity indices that are invariant to monotonic transformation of the output.

In this work, we investigate in detail the implications of invariance for monotonic transformations (henceforth, monotonic invariance) in the estimation of global sensitivity statistics. First, we propose a general framework for monotonic invariant global sensitivity statistics. We argue that any global sensitivity measure be seen as a functional of the unconditional model output distribution and of the conditional model output distribution obtained when any given factor is fixed. Then, we investigate the nature of monotonic invariance showing that one can obtain monotonic invariant global sensitivity statistics choosing a proper probability metric. We propose a generalized variational distance which encompass several monotonic invariant probability metrics. We show that the Kuiper, Kolmogorov, Anderson-Darling, the L^1-norm, any Csiszar-divergence [1, 5, 9, 2] and any member of the Birnbaum-Orlicz family [3] generate monotonic invariant global sensitivity statistics. Also, the estimation of the sensitivity statistics becomes equivalent to a sequence of repeated goodness of fit tests.

The numerical implications of transformation invariance are addressed next. We illustrate numerical experiments through both analytical case studies and through the Level E model, used in [7], which is a benchmark model for global sensitivity analysis studies. We compare results for statistics that are monotonic invariant and statistics that are not monotonic invariant. To test the independence of results from the estimation method, alternative estimation strategies are analysed for the same sensitivity statistic.

Results show that, if an appropriate monotonic transformation is employed, the rate of convergence with respect to the sample size increases for both invariant and non-invariant sensitivity statistics. The transformation allows one to obtain stable estimates in cases in which it would otherwise be impossible to obtain convergence. However, for sensitivity statistics that are not monotonic invariant the results can be distorted and misleading, i.e. different transformations may yield a different ranking of factors. If a sensitivity statistic is monotonic invariant, then we fully retain the increased computational accuracy.

DISCLAIMER: an extended version of the manuscript is presently under review at an internation-

ally refereed journal.

References:

[1] T. W. Anderson and D. A. Darling. Asymptotic theory of certain "goodness of fit" criteria based on stochastic processes. *Annals of Mathematical Statistics*, 23(2):193–212, 1952.

[2] I. Csiszár and P. Shields. Information theory and statistics: A tutorial. *Foundations and Trends in Communications and Information Theory*, 1(4):417–528, 2004.

[3] E. Deza and M. M. Deza. *Dictionary of Distances*. Elsevier, Amsterdam, 2006.

[4] J. E. Oakley and A. O'Hagan. Probabilistic sensitivity analysis of complex models: A Bayesian approach. *J. R. Statist. Soc. B*, 66(3):751–769, 2004.

[5] E. S. Pearson. Comparison of tests for randomness of points on a line. *Biometrika*, 50(3/4):315–325, 1963.

[6] H. Rabitz and Ö. F. Alış. General foundations of high-dimensional model representations. *J. Math. Chem.*, 25(2–3):197–233, 1999.

[7] A. Saltelli and S. Tarantola. On the relative importance of input factors in mathematical models: Safety assessment for nuclear waste disposal. *J. Amer. Statist. Assoc.*, 97(459):702–709, 2002.

[8] A. Saltelli, S. Tarantola, and F. Campolongo. Sensitivity analysis as an ingredient of modelling. *Stat. Sci.*, 19(4):377–395, 2000.

[9] M. Tygert. Statistical tests for whether a given set of independent, identically distributed draws comes from a specified probability density. *PNAS*, 107(38):16471–16476, 2010.

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Covariance-based sensitivity indices based on polynomial chaos functional decomposition

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The art of robust engineering requires to take the random nature of design parameters into account in order to predict the dispersion of the performance of a structure. When dealing with reducing this dispersion, one has to identify the parameters to which the variability of the performance is the most sensitive. Global sensitivity analysis (GSA) is a statistical field that aims at identifying and prioritizing the design parameters that contribute the most to the dispersion of the response of a model. This quantity is in most cases described by the statistical variance of the model response. The so-called ANOVA (ANalysis Of VAriance) technique ranks the parameter according the share of the model response variance they are responsible for.

Let us consider a performance Y described by a physical model $\mathcal{M}(\boldsymbol{X})$ where $\boldsymbol{X}$ is $n-$dimensional independent random vector. Such an apportionment of the total variance can be processed thanks to a functional decomposition of the model $\mathcal{M}$ [1] reading:

$$\begin{aligned}\mathcal{M}(\boldsymbol{X}) &= \mathcal{M}_0 + \sum_{i=1}^{n} \mathcal{M}_i(X_i) + \sum_{1\leqslant i<j\leqslant n} \mathcal{M}_{ij}(X_i, X_j) + \cdots + \mathcal{M}_{1\ldots n}(X_1, \ldots, X_n) \\ &= \mathcal{M}_0 + \sum_{\boldsymbol{u}\subseteq\{1,\ldots,n\}} \mathcal{M}_{\boldsymbol{u}}(\boldsymbol{X}_{\boldsymbol{u}})\end{aligned} \tag{1}$$

where $\mathcal{M}_0$ is a constant and where the components have zero mean and are mutually orthogonal. This decomposition also holds when dealing with the variance of Y:

$$\mathbb{V}[Y] = \sum_{i=1}^{n} \mathbb{V}[\mathcal{M}_i(X_i)] + \sum_{1\leqslant i<j\leqslant n} \mathbb{V}[\mathcal{M}_{ij}(X_i, X_j)] + \cdots + \mathbb{V}[\mathcal{M}_{1\ldots n}(X_1, \ldots, X_n)] \tag{2}$$

The so-called Sobol' index [2] of a variable X_i is defined by the ratio between the variance of the component that only depends on X_i and the total variance of Y, namely:

$$S_i = \frac{\mathbb{V}[\mathcal{M}_i(X_i)]}{\mathbb{V}[Y]} \tag{3}$$

The index S_i represents the share of the variance of Y that is due to both the physical role of X_i in $\mathcal{M}$ and its random nature. An index S_i close to 1 indicates a strong contribution of X_i to the dispersion of Y whereas an index close to 0 denotes a weak incidence.

Computing the ANOVA sensitivity indices requires to identify the different components of the functional decomposition. This task can be achieved by a projection method but the corresponding computational cost is substantial. On top of that, if the response of the model $\mathcal{M}$ is expensive to evaluate (if $\mathcal{M}$ is a FEM code for instance), then the number of calls to the model will be limited, let us say to a few hundreds of times, which is not sufficient to perform GSA. In order to circumvent this limitation, one may substitute the physical model by a surrogate model $\widehat{\mathcal{M}}$, namely a analytical representation built from a reasonable-sized design of experiment $\mathcal{D} = \{\boldsymbol{\mathcal{X}}, \mathcal{Y} = \mathcal{M}(\boldsymbol{\mathcal{X}})\}$ that is much cheaper to evaluate than $\mathcal{M}$. One adequate method is referred to as polynomial chaos expansion [3]. The principle is to expand the model response on a suitable polynomial basis, namely:

$$Y \approx \widehat{\mathcal{M}}(\boldsymbol{X}) = \sum_{j=0}^{+\infty} a_j \Psi_j(\boldsymbol{X}) \tag{4}$$

In practice, the basis $\mathcal{B} = \{\Psi_j,\, j = 0, \ldots, P-1\}$ is usually truncated to a finite number P of terms. Then, defining a substitution model for $\mathcal{M}$ consists in evaluating the coefficients a_j of the development, using a regression method for instance.

GSA techniques for models with independent input parameters are well-established and computationally efficient when coupled with surrogate models. When the input parameters are no longer independent, the functional decomposition in (1) does not hold since the components of the decomposition are no longer orthogonal. A generalization of the ANOVA for models with correlated input has been introduced in [4]. The principle of the ANCOVA (ANalysis of COVAriance) is to express the variance of Y as its covariance with the functional decomposition of $\mathcal{M}$, namely:

$$\begin{aligned}\mathbb{V}[Y] &= \mathbb{C}[Y, \mathcal{M}(\boldsymbol{X})] \\ &= \mathbb{C}\left[Y, \sum_{\boldsymbol{u}\subseteq\{1,\ldots,n\}} \mathcal{M}_{\boldsymbol{u}}(\boldsymbol{X}_{\boldsymbol{u}})\right] \\ &= \sum_{\boldsymbol{u}\subseteq\{1,\ldots,n\}} \left[\mathbb{V}[\mathcal{M}_{\boldsymbol{u}}(\boldsymbol{X}_{\boldsymbol{u}})] + \mathbb{C}[\mathcal{M}_{\boldsymbol{u}}(\boldsymbol{X}_{\boldsymbol{u}}), Y - \mathcal{M}_{\boldsymbol{u}}(\boldsymbol{X}_{\boldsymbol{u}})]\right]\end{aligned} \tag{5}$$

The following triplet of indices $(S_{\boldsymbol{u}}, S^U_{\boldsymbol{u}}, S^C_{\boldsymbol{u}})$ can be derived from (5):

$$S_{\boldsymbol{u}} = \frac{\mathbb{C}[\mathcal{M}_{\boldsymbol{u}}(\boldsymbol{X}_{\boldsymbol{u}}), Y]}{\mathbb{V}[Y]}, \quad S^U_{\boldsymbol{u}} = \frac{\mathbb{V}[\mathcal{M}_{\boldsymbol{u}}(\boldsymbol{X}_{\boldsymbol{u}})]}{\mathbb{V}[Y]}, \quad S^C_{\boldsymbol{u}} = S_{\boldsymbol{u}} - S^U_{\boldsymbol{u}} \tag{6}$$

The index $S^U_{\boldsymbol{u}}$ represents the uncorrelated contribution of $\boldsymbol{X}_{\boldsymbol{u}}$ to the variance of Y, that the contribution that would be left if the variables where independent. On the contrary, the index $S^C_{\boldsymbol{u}}$ represents the contribution of the correlation of $\boldsymbol{X}_{\boldsymbol{u}}$ with the other parameters. The global contribution index $S_{\boldsymbol{u}} = S^U_{\boldsymbol{u}} + S^C_{\boldsymbol{u}}$ is the sum of the two contributions.

The issue of the functional decomposition is solved by using the one provided by the polynomial chaos expansion in (4). Since the expansion of the correlated parameters is not expressed in the physical space because of the isoprobabilistic transformation, the *trick* proposed in [5] is to build the expansion with the joint distribution of the input random vector $\boldsymbol{X}$ featuring an independent copula to preserve the link between the physical and standard variables and to evaluate the variances and covariances by simulating realizations of $\boldsymbol{X}$ with its true dependence structure.

The ANCOVA technique coupled with polynomial chaos expansion is first applied on analytical test functions in order to exhibit how the uncorrelated an correlated parts behave when the correlation between the input parameters varies. It is then carried out on a simple mechanical application.

References:

[1] W. Hoeffding, "A class of statistics with asymptotically normal distributions", *Annals of Statistics*, **19**:293–325, 1948.

[2] I.M. Sobol', "Sensitivity estimates for nonlinear Mathematical models", *Matem. Modelirovanie*, **2**(1):112–118, 1990 (in Russian), *MMCE*, **1**(4):407–414, 1993 (in English).

[3] B. Sudret, "Global sensitivity analysis using polynomial chaos expansions", *Reliab. Eng. Sys. Safety*, **93**:964–979, 2008.

[4] G. Li and H. Rabitz, "Global Sensitivity Analysis for Systems with Independent and/or Correlated Inputs", *J. Phys. Chem.*, **114**:6022–6032, 2010.

[5] Y. Caniou, "Global sensitivity analysis for nested and multiscale modelling", Université Blaise Pascal – Clermont II, 2012.

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Assessing the robustness of sensitivity analysis results. Application to traffic simulation models

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In recent time, in the field of traffic simulation, sensitivity analysis (SA) is starting to attract attention as an indispensible tool for simplifying the calibration of microscopic traffic flow models (*1*,*2*,*3*). These models, in facts, involve many sub-models and dozens of parameters (*4*) that need to be calibrated to make the model suitable to correctly reproduce local traffic conditions. Unfortunately, such models are quite computationally expensive (the typical duration of a simulation run being in the order of minutes) meanwhile the calibration in the high-dimensional space of model parameters usually requires several thousands of model evaluations. For this reason, it is common practice to carry out calibration only for a limited number of parameters. However, there is no established procedure for their selection, other than the personal experience. Therefore it is easy to imagine as the selection of an incomplete set of parameters for the calibration might lead to several issues, including but not limited to the inaccuracy and unreliability of model results as well as unrealistic values for the calibrated parameters. Therefore, a proper SA, including the initial screening of the parameters, can be very valuable for the subsequent calibration process (*5*), as it can provide both quantitative and qualitative information regarding the effects of the different model parameters (and their variations) on the simulation results.

The sensitivity analysis of traffic simulation models is therefore carried out on its parameters, whereas the other inputs like the transportation network or the travel demand are kept constant. Since many sensitivity analysis techniques require a considerable number of model evaluations (*5*) and a SA needs to be repeated for each specific case study, the computational complexity still remains a problem. For this reason, the possibility of generalizing results of a SA of a specific traffic simulation model in a specific case study, is worth to be investigated.

In the present work we present the preliminary results of an exploratory research in which the robustness of the results of a sensitivity analysis, carried out on the parameters of a car-following model, is assessed against the variation of the other (non-parametric) inputs.

Car-following models are the key components of all microscopic traffic simulation models. They describe the longitudinal motion of a vehicle by mimicking the reaction of its driver (the "follower") to the stimuli perceived while interacting with the front vehicle (the "leader"). They are in the form of differential equations (sometimes delayed) whose basic inputs are, generally, the follower's speed, the distance between the follower and the leader and their speed difference. Outputs of such models are usually the follower's speed or acceleration. Traffic is therefore simulated through a system of chained coupled equations.

Apart from the mentioned inputs, simulation outputs are strongly dependent on the values of the model parameters , which vary among the population of drivers (that is along the chain of coupled equations) as deemed to capture the individual psycho-physical characteristics of each driver. In simulation practice such parameters are considered uncertain in order to cover all the uncertainty in the simulation process. They are usually calibrated through an inverse analysis, that is by looking for the value of parameters that allow the simulated time-space trajectory of a vehicle to be as near as possible to the measured one.

Although these models have usually a quite simple formulation, their behavior, especially as the result of the parameter values, is not yet clear. Their SA is therefore an interesting and timely issue. As already mentioned, however, this is not the only objective of this work. Here, we do want also to

ascertain how robust are the results of the analysis against the variation of the non-parametric inputs, that is, by varying the *leader's trajectory*. To this aim, the sensitivity analysis included the leader's trajectory as an additional factor, which, in the Monte Carlo framework adopted, was sampled from a predefined dataset of trajectories. Such dataset, in particular, was built by picking trajectories measured in different roads (freeway and arterial) and in different traffic conditions. In this way it was possible to assess the relative effect on model outputs of the parameters and the input trajectories that was essential to understand whether results of a SA can be generalized (independently of the trajectory).

In the experiment, we chose the sensitivity analysis technique based on the computation of the Sobol first order and total order sensitivity indices (*5*,*6*). Confidence intervals around the indices were also calculated in order to check for their stability. The car-following model used was the IDM model, while the trajectories considered were 101 trajectories selected from 10 databases available thanks to the NGSIM project which allowed us to capture a wide spectrum of driving behaviors. Some results are summarized in Figure 1.

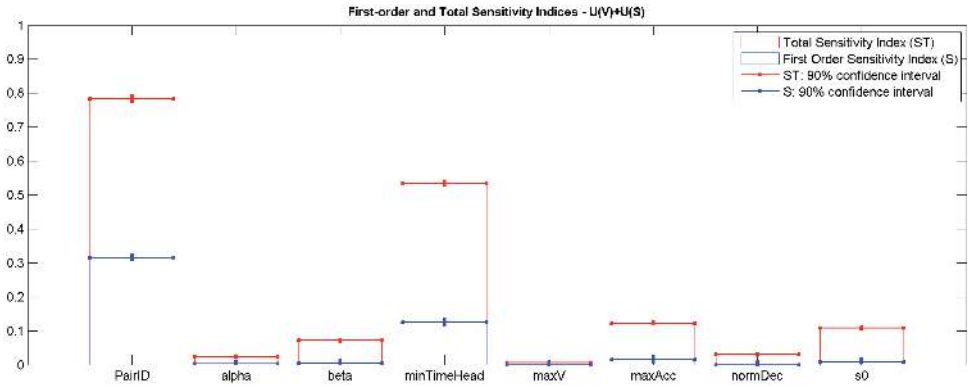

Figure 1. First and total order sensitivity indices for the parameters of the IDM model.

They show that the input trajectory (identified by the *PairID* variable) has a prominent effect on the model outputs. At the same time, however, its effect is mainly played in combination with other model parameters. Overall, it can be said that there are few parameters exerting a certain effect on the output of the model no matter the input used. This is an important result as it opens the path for defining classes of problems, in traffic simulation, for which the parameters to calibrate can be defined a priori and not individuated case by case.

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References :

1. Punzo, V., and B. Ciuffo. How parameters of microscopic traffic flow models relate to traffic conditions and implications on model calibration. In *Transportation Research Records*, No. 2124, 2009, pp. 249 - 256.
2. Punzo, V., and Ciuffo, B. Sensitivity Analysis of Car-following Models: Methodology and Application. In *Proceedings of the 90th TRB Annual Meeting*, Washington DC, 2011.
3. Ge, Q., and M. Menendez. An improved approach for the sensitivity analysis of computationally expensive microscopic traffic models: a case study of the Zurich network in VISSIM. *92th TRB Annual Meeting*, Washington DC, 2013.
4. Ciuffo, B., Lima Azavedo, C. Multistep Approach for Global Sensitivity Analysis of Complex Traffic Simulation Models: Application to MITSIM Model. *92th TRB Annual Meeting*, Washington DC, 2013.
5. Saltelli, A.; Ratto, M.; Anres, T.; Campolongo, F.; Cariboni, J.; Gatelli, D.; Saisana, M.; Tarantola. S.; *Global Sensitivity Analysis – The Primer*; John Wiley and Sons Ltd: Cheichester, England, 2008.
6. Saltelli, A., Annoni, P., Azzini, I., Campolongo, F., Ratto, M., Tarantola, S. Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index. In *Computer Physics Communications*, vol. 181, pp. 259-270. 2010

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A class of ANOVA kernels dedicated to sensitivity analysis

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Motivation : The aim of global sensitivity analysis is to describe the inner structure of a real-valued function f of several variables, and to analyse the influence of each (group of) variable(s) on the response. It is based on the High Dimensional Model Representation (HDMR) of f [2]:

$$f(x) = f_0 + \sum_{i=1}^{d} f_i(x_i) + \sum_{i<j} f_{i,j}(x_i, x_j) + \cdots + f_{1,\ldots,d}(x) \tag{1}$$

where the integrals of f_I ($I \subset \{1, ..., d\}$) with respect to any of its variable are equal to zero[1].

Computing the various f_I terms requires to integrate f multiple times (and potentially over large dimensional spaces), so that it cannot be performed directly when evaluations of f are costly. A popular alternative is to perform the sensitivity analysis on an mathematical model m that approximates f. We show that when m is based on Gaussian process regression with a kernel from an appropriate class, the HDMR of m can be obtained in a very convenient way.

Results: This work corresponds to a recently published article [1]. Let us introduce the kernel

$$K^*_{ANOVA}(x, y) = \prod_{i=1}^{d} \left(1 + k_i^0(x_i, y_i)\right) = \sum_{I \subset \{1,\ldots,d\}} \prod_{i \in I} k_i^0(x_i, y_i) = \sum_{I \subset \{1,\ldots,d\}} k_I^0(x_I, y_I) \tag{2}$$

where the kernels k_i^0 are associated to reproducing kernel Hilbert spaces (RKHS) of zero mean functions for μ_i. The ANOVA structure of K^*_{ANOVA} allows to decompose the best predictor of the associated Gaussian process model in a sum of sub-models:

$$m(x) = k(x)^t K^{-1} Y = m_0 + \sum_{i=1}^{d} m_i(x_i) + \sum_{i<j} m_{i,j}(x_i, x_j) + \cdots + m_{1,\ldots,d}(x) \tag{3}$$

where $m_I(x_I) = k_I^0(x_I)^t K^{-1} Y$. Furthermore, one can associate the prediction variance $v_I(x) = k_I(x_I, y_I) - k_I(x_I)^t K^{-1} k_I(x_I)$ to each submodel m_I. Let us remark, however, that the sum of the variances of the sub-models does not coincide with the variance of the full model.

A striking fact with K^*_{ANOVA} kernels is that the decomposition given by eq. 3 coincides with the HDMR of m since, by construction, the sub-models correspond to the projections of m onto sub-spaces of zero-mean functions. As a consequence, the HDMR of the model can be obtained at any order without the need to compute high dimensional integrals. Note that this construction is similar to SS-ANOVA [3] but the framework is more general here since we do not focus on splines.

[1] Note that we assume here an input space of the form $D = D_1 \times \cdots \times D_d$ endowed with a product measure $\mu = \mu_1 \otimes \cdots \otimes \mu_d$.

Another contribution of [1] is to show how to obtain kernels associated to RKHS of zero-mean functions. Let k be a kernel and $\mathcal{H}$ be the associated RKHS. Under the hypothesis $\int_{D_i} k_i(s_i,s_i)\,\mathrm{d}\mu_i(s_i) < \infty$, the kernel k_i^0 associated to the sub-space of zero-mean functions in $\mathcal{H}$ is

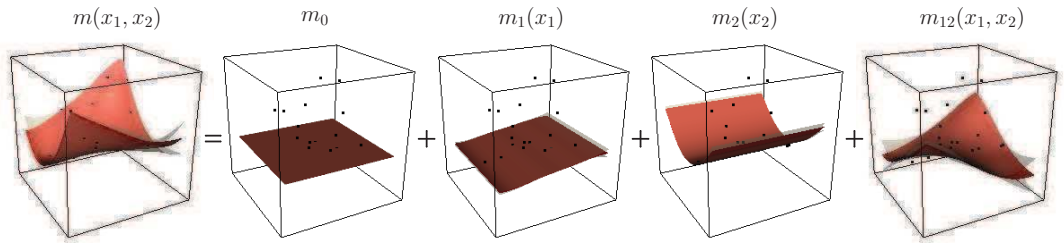
$$k_i^0(x_i,y_i) = k_i(x_i,y_i) - \frac{\displaystyle\int_{D_i} k_i(x_i,s_i)\,\mathrm{d}\mu_i(s_i) \int_{D_i} k_i(y_i,s_i)\,\mathrm{d}\mu_i(s_i)}{\displaystyle\iint_{D_i^2} k_i(s_i,t_i)\,\mathrm{d}\mu_i(s_i)\mathrm{d}\mu_i(t_i)}. \tag{4}$$

We finally show that the global sensitivity indices S_I of m^* are given by:

$$S_I = \frac{Y^t K^{-1}\big(\bigodot_{i\in I}\Gamma_i\big)K^{-1}Y}{Y^t K^{-1}\big(\bigodot_{i=1}^d(1_{n\times n}+\Gamma_i)-1_{n\times n}\big)K^{-1}Y} \tag{5}$$

where Γ_i is the $n\times n$ matrix $\Gamma_i = \int_{D_i} k_i^0(s_i)k_i^0(s_i)^t\,\mathrm{d}\mu_i(s_i)$ and $1_{n\times n}$ is the $n\times n$ matrix of ones. Compared to the similar property given in [4], the particular structure of K^*_{ANOVA} allows here to compute the indices S_I at any order without the need to compute all S_J for $J\subset I$.

Illustration: In order to illustrate briefly the previous results we consider the test function $f(x) = x_1 + x_2^2 + x_1x_2$ defined on $[-5,5]^2$. Given evaluations of f on a 10-point LH design we build a model based on a K^*_{ANOVA} kernel. Its decomposition in sub-models can be represented as



The computation of the sensitivity indices on m gives $S_1 = 0.23$, $S_2 = 0.48$, $S_{12} = 0.29$, a reasonably good approximation of the true values: $S_1 = 0.25$, $S_2 = 0.5$ and $S_{12} = 0.25$.

References:

[1] N. Durrande, D. Ginsbourger, O. Roustant and L. Carraro, "ANOVA kernels and RKHS of zero mean functions for model-based sensitivity analysis", *J. of Multi. Anal.*, **155**:57–67, 2013.

[2] I.M. Sobol, "Theorems and examples on high dimensional model representation", *Reliability Engineering & System Safety*, **79**(2):187–193, 2003.

[3] C. Gu, "Smoothing spline ANOVA models", Springer Verlag, 2002.

[4] W. Chen, R. Jin, and A. Sudjianto, "Analytical variance-based global sensitivity analysis in simulation-based design under uncertainty", *Journal of mechanical design*, **127**:875–886, 2005.

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Bayesian estimates of the parameter variability in turbulence models for the RANS equations.

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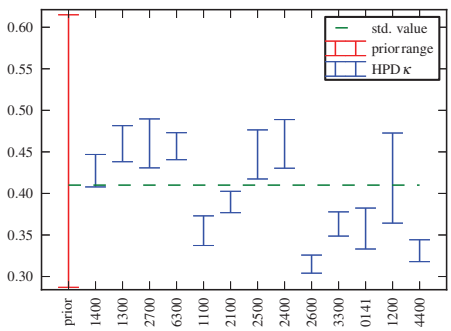
Computational Fluid Dynamics (CFD) simulations represent a key element of the analysis and design methods used in industry. These simulations are typically based on a unique set of input data and model parameters. However, real-world flow configurations are subject to numerous uncertainties, e.g. variations in boundary and initial conditions. The presence of these uncertainties is a major source of error in the design decision process and increases the risk of failure of a given component. The proposed research work focuses on the quantification of modeling uncertainties using a statistical approach.

An essential ingredient in CFD simulation is represented by turbulence modeling. Capturing all the spatial and temporal scales on a computational grid, is typically not feasible considering the currently available computing power. In current CFD practice, all the turbulent scales are modeled, and only the average flow field is solved directly. This is known as the Reynolds-Averaged Navier-Stokes (RANS) framework [1]. The averaging process of the Navier-Stokes equations leads to the appearance of additional terms, resulting in an unclosed system. RANS approaches tackle this problem by introducing additional constitutive models, i.e. turbulence models, which come with their own mathematical structure and closure parameters.

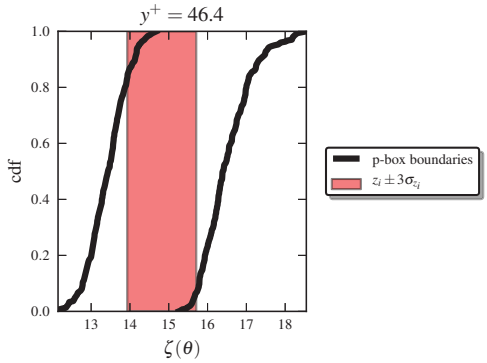
Within the framework of the RANS equations, several turbulence models are available in the literature (see e.g. Ref. [1] for a review). There is a quite general agreement about the fact that no universal turbulence model exists, i.e. the performance of different turbulence models is strongly problem-dependent [2]. Moreover, a specific turbulence model uses a number of closure coefficients which are traditionally determined by calibrating the model for a dataset of relatively simple test cases. The model performance may strongly depend on the selected coefficients, which are often re-calibrated to improve the model response for a given set of problems.

For calibration, we follow the work of Cheung et al. [3], in which a Bayesian approach was applied to the calibration of a well-know turbulence model. In that work, the coefficients were calibrated once on all the available measured velocity profiles and wall-shear stress components. Model inadequacy was treated with a multiplicative term parameterized in the wall-normal direction with a Gaussian process, following the framework of Kennedy and O'Hagan [4]. The latter authors define model inadequacy as the discrepancy remaining between the mean of the real-world process and the model evaluated at the 'true' parameters. These parameters are defined as those values who give a best-fit to the data under the assumed form of the statistical model. Thus, even when we assume that we know these best-fit closure coefficients, assumptions intrinsic to the mathematical structure of the turbulence model will prevent it from reproducing a Quantity of Interest without error.

In the present work, we perform the calibrations on a set of popular turbulence models. Unlike Cheung, we quantify model inadequacy using multiple calibration results. Summarized we proceed as follows: (1) we define the class of flows for which we wish to estimate the error, in our case turbulent boundary-layers for a range of pressure gradients. (2) We collect experimental data for a number of flows of this class. (3) We use Bayesian model updating to calibrate the closure coefficients against each flow in this data-set, resulting in posterior distributions on the coefficients for each flow. We obtain samples from these distributions by running a boundary-layer code in the Markov-Chain Monte-Carlo (McMC) method. Thanks to the low-computational cost of the boundary-layer code (less than 1 second / simulation), McMC sampling does not require the use of surrogate models and is coupled directly to the exact model. The Markov chains are found to converge after approximately 35.000 samples, and statistics are computed on 5.000 sam-



(a) The prior range and the posterior HPD intervals for the 13 flow cases.



(b) The p-box at a given normalized y station. The shaded area is the region of experimental uncertainty.

ples. (4) We summarize the large amount of posterior information using Highest Posterior-Density (HPD) intervals. This summary gives most-likely intervals on the coefficients which represent both the spread of coefficients within the flow-class, as well as the ability of the calibration to provide information about the values these coefficients should take in each individual flow case. Figure (a) shows the HPD intervals of one of the parameters, namely the von Karman constant κ, which are quite well informed by the calibrations. This was to be expected, since a sensitivity analysis based on Sobol indices [5] showed κ is a sensitive input parameter. (5) For a new flow of the class (i.e. a new pressure gradient), for which there might be no experimental data, we perform a simulation in order to obtain probabilistic error bars on the model output. Our approach is to construct a probability box (p-box) for the output of the model at the new pressure gradient, using uniformly distributed sets of coefficients bounded by the HPD intervals of the 13 calibrated cases. We propagate each of these coefficient sets through the model to obtain 13 random variables Z_k, where each one represents the posterior uncertainty of a calibrated flow case k on the model output at the new pressure gradient. Next we calculate an approximate cumulative-density function (cdf) for each Z_k. The envelope formed by this collection of cdfs is called a p-box, of which an example is depicted in Figure (b). To construct a worst-case 90% credible interval on the model output we find the model output value of the left p-box boundary corresponding to a 0.05 probability content, and the value with a 0.95 probability content from the right boundary.

At the conference we will show the mentioned results for all turbulence models in the considered set, and also compare how much the quality of each model's predictions depends upon the inclusion of a model inadequacy term. Alternatively, comparisons of the posterior plausibility associated with each turbulence model (evaluated at the different flow cases) will also allow for conclusions to be reached on the possible existence of a single 'best model' for the class of flows under consideration.

References:

[1] Wilcox, D.C., "Turbulence modeling for CFD, Third ed.", DCW industries La Canada
[2] Zhang, Z. et. al. , "Evaluation of various turbulence models in predicting airflow and turbulence in enclosed environments by CFD: Part 2", *Hvac&R Research*, **13**: 871–886 (2007)
[3] Cheung, S.H. et. al. , "Bayesian uncertainty analysis with applications to turbulence modeling", *Reliability engineering and systems safety*, **96**: 1137–1149 (2011)
[4] Kennedy, M.C. et. al. , "Bayesian calibration of computer models", *J. of the Roy. Stat. Society: Series B*, **63**: 425–464 (2001)
[5] Tang, G. et. al. "Global sensitivity analysis for stochastic collocation expansion", *CSRI summer proceedins 2009*

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Simple and efficient tools to explore complex models in agroecology with an eye on interactions

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Sensitivity analysis and model exploration require flexible sampling and analysis tools. In biology and agroecology applications, they must cope with many possible types of model features, including stochasticity, interactions, mixtures of qualitative and quantitative factors, crossed and nested input factors, etc. In this talk, we advocate methods that are based on standard statistical methodology but integrate the modern approaches to model exploration. More precisely, we show how a combination of regular factorial designs and regression-based metamodelling techniques can be adapted to generate flexible space-filling designs and to explore the main effects and interactions of the input factors.

From our experience, most of the models developped in agroecology have two main characteristics. The first one is that a small number of input parameters explain most of the variability of the model outputs ; the second one is that most of the input parameters have a strong linear or polynomial main effect with a limited order of interactions.

The basic metamodel we postulate to explore the models is a polynomial linear model of a low degree D (typically, $D = 3$ at max.). Interactions are modelled by products of powers of input parameters, with the constraint that the sum of these powers is lower than or equal to D. The plmm, for polynomial linear metamodel, corresponds to the model

$$Y = \sum_{a=1}^{A} \beta_a \left(\prod_{k=1}^{K} X_k^{d_{a,k}} \right) + \eta$$

where K is the number of input parameters; $A = C_{K+D}^{D}$ is the number of cross product terms that satisfy $0 \leq \sum_k d_{a,k} \leq D$, with D the maximal degree of the polynomial; η is a centred random term independent of the X_k variables.

The coefficient of determination R^2 expresses the percentage of variation explained by a regression model (see Saporta, 2011 among others). With such an index, it is possible to evaluate the specific contribution of each input parameter, alone or in interaction with other parameters.

Three R^2 values are needed to evaluate the contributions of a parameter.

The first one (R_C^2) is the coefficient of determination of the complete model. It gives the total percentage of variation explained by the A terms in the complete model: $1 - R_C^2$ corresponds to the part not explained by such a polynomial linear model and so to the random term η.

The second one (R_k^2) corresponds to the main effect of the parameter X_k, assuming all other terms are negligible: it is evaluated by the coefficient of determination of the polynomial model that involves the single input parameter X_k. It can be considered as an (estimated) upper bound of the actual main effect of X_k, because it is not adjusted with respect to the other parameters.

R_{-k}^2 is the coefficient of determination of the plmm when input parameter X_k is not taken into account.

With these three values, the total contribution of the parameter X_k (main effect and interactions with other parameters) is evaluated by $R_C^2 - R_{-k}^2$. It corresponds to the classical Total sensitivity index under the assumption that the plmm is the true model.

In principle, the difference Δ between $R_C^2 - R_{-k}^2$ and R_k^2 can be used to quantify the interactions between parameter X_k and others. However it is also influenced by correlations and confounding

between explanatory variables (two parameters may explain the same model output variation). Notice that Δ can be negative when confounding occurs, which arises frequently if the experimental design is not balanced (with respect to the information matrix).

To better estimate interaction, it is necessary to reduce confounding through appropriate sampling designs. Several types are available for sensitivity analysis (LHS, regular fractional design, Sobol' sequences, . . .). We focus on the scrambled (t, m, s)-net designs (see Koehler and Owen, 1996), which satisfy the properties of Latin hypercubes together with space filling properties in dimensions greater than 1. We explore their potential on some models developped in agroecology and compare it to other designs when estimating parameters' contributions to the model output variation using plmm.

To gain insight, we discuss the relationship between (t, m, s)-net designs and regular fractional designs based on defining relationships (Dey and Mukerjee, 1999, Pistone and Rogantin, 2008). Based on the recent Planor R package (Monod, Kobilinsky and Bouvier, 2012), we show how the (t, m, s)-net type of design can be tailored to make the effects of interest estimable assuming a given polynomial model on the input factors.

The talk is illustrated by the exploration of some standard models and of agroecological models.

References:

A. Dey and R. Mukerjee, "*Fractional Factorial Plans*", Wiley Series in Probability and Statistics, 1999.

J.R. Koehler and A.B. Owen, "Computer experiments", *in* S. Ghosh and C.R. Rao eds, *Handbook of Statistics* **13**, 261–308, Elsevier Science B.V., Amsterdam, 1996.

H. Monod, A. Bouvier and A. Kobilinsky, "A quick guide to PLANOR, an R package for the automatic generation of regular fractional factorial designs", CRAN, 2012.

G. Pistone and M.-P. Rogantin, Indicator function and complex coding for mixed fractional factorial designs. *Journal of Statistical Planning and Inference*, 138(3):787-802, 2008.

G. Saporta, *Probabilité, Analyse des Données et Statistique*, Technip, Paris, 3rd edition, 2011.

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Revisiting Morris Method: a polynomial algebra for design definition with increased efficiency and observability

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Morris scheme for One At a Time (OAT) designs for sensitivity analysis [1] is widely used for rapid identification of the groups of important (further classified into linear or mixed/non-linear) and unimportant inputs of a multivariate function $f(x), x \in A \subset \mathbb{R}^k$, and is particularly relevant for models whose execution is computationally expensive and time consuming [2].

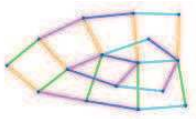
Morris designs are restricted to points in a finite k-dimensional grid $\mathcal{G} \subset A$ covering the domain of f. Stated in simple terms, the method starts by randomly evaluating $f(\cdot)$ at r "initial points" $\{x^{(n)}\}_{n=1}^r$ in $\mathcal{G}$. Starting at each of these r points, say $x^{(n)}$, k successive evaluations of $f(\cdot)$ are made, each two consecutive points enabling the determination of an elementary effect $EE_i^{(n)}$ along a distinct direction $i \in \{1, \ldots, k\}$. Morris designs are thus composed of r paths in $\mathcal{G}$ of size $k+1$, which do not have two segments along the same direction. Each input factor x_i is then classified as irrelevant, linear or other (non-linear or involved in cross-effects), depending on the first and second order statistics of the set of elementary effects $\{EE_i^{(n)}\}_{n=1}^r$ observed. The attractiveness of Morris Elementary Effects method relies on the fact that the size of the designs required to detect the important input factors of $f(\cdot)$ is linear in the number of input factors (being equal to $r(k+1)$) irrespective of the resolution of the grid $\mathcal{G}$, providing an efficient initial screening of the sensitivity of $f(\cdot)$ with respect to each input factor.

Given its higher efficiency, the clustered version of Morris OAT designs (see [1], Section 5), that computes $m > 1$ Elementary Effects $\{EE_i^{(j)}(x)\}_{j=1}^m$ along all directions $i = 1, \ldots, k$ of the input space in the neighbourhood of each point $x^{(n)}$, is especially appealing. Surprisingly, these more complex designs seem to have attracted much less interest than the original ($m = 1$) version. Possible reasons are the lack of a constructive method for finding these designs, and, presumably, concerns about the impact of residual correlation amongst the resulting set of elementary effects along each direction, see [4].

In this communication we complete the original presentation of Morris [1], giving a formal specification of a family of balanced clustered designs for arbitrary values of k and $m \leq 2^{k-1}$ (Morris construction is valid only for pairs (k, m) where k is not prime and m is a divisor of k). Our construction is supported on the definition of an isometry between sub-graphs of the unit cube Q_k equipped of the Manhattan metric, and a set of polynomials in $(x_1, \ldots, x_k)$ on which a convenient inner product is defined. This isometry, based on the association $(s_i)_{i=1}^d \in Q_d \hookrightarrow X_1^{s_1} \cdots X_d^{s_d}$, enables explicit symbolic representation and manipulation of designs, as well as the formal demonstration of their properties. We define (k, m)-edge balanced designs as those that enable the determination of exactly m elementary effects for each direction. Using our polynomial representation this is equivalent to finding the polynomial solutions to a set of equations. The computation of the set of elementary effects provided by any given subgraph is then immediate using our polynomial representation, even if the designs are no longer OAT.

A natural but more complex algebra over the set of polynomials also enables the extension of Morris concept of clustered designs to the estimation of two-factor interaction effects, $SEE_{ij}(x), i \neq j \in \{1, \ldots, k\}$, that can detect the presence of products $x_i x_j$ of pairs of input factors. We define (k, c)-cycle balanced designs as the subgraphs of the unit hypercube Q_k that are (k, m)-edge balanced for some m and contain exactly c 4-cycles in direction (i, j) all $k(k-1)/2$ possible pairs. In the paper we present the system of equations that define these designs. For $c = 1, 2$ and 3 we present families of (k, c)-cycle balanced designs, that are recursively defined in terms of their polynomial representations. The figure below shows a $(5, 1)$-cycle balanced solution, together with the recursive

equations that define the family for $c = 1$. In this Figure, edges are coloured according to the elementary effect that is computed from their end points, there are thus 5 distinct colors. The graph represents a $(5, 1)$-cycle balanced design because there is exactly one cycle of dimension 4 involving all 10 possible pairs of colors.



$$G_1^1 = 1 + X_1, \qquad G_2^1 = G_1^1 + X_2 G_1^1,$$
$$G_3^1 = G_2^1 + X_3\,(1 + X_1 + X_2)\,, \qquad G_4^1 = G_3^1 + X_4\,(1 + X_1 + X_2 + X_3)$$
$$G_5^1 = G_3^1 + X_5\,(1 + X_1 + X_2 + X_3 + X_4) \qquad \cdots$$

Our work is related to a previously proposed "New Morris method", see [6,7]. However, these references only consider the case $c = 1$, i.e., computation of a single mixed effect for each pair of input factors and do not impose that the resulting designs are edge balanced.

We show how our approach can formally be extended to sampling of higher order derivatives by imposing the presence of certain patterns in the designs graphs.

Explicit formulas for the size of our edge and cycle balanced designs are provided, and we compare their economy (defined as in [1], as the ratio of the number of effects computed over the size of the design) to the economy of the original and New Morris methods. The performance of cycle balanced designs is demonstrated by considering both the analytical function on Morris' original paper [1] and a true simulation model of a complex system with a large number of inputs.

Finally, we discuss the problem of finding designs able to detect n-th order terms in each input factor, which requires definition of a suitable isometry between $\{0, \ldots, n\}^k$ and polynomials.

References:

[1] Max D. Morris, "Factorial Sampling Plans for Preliminary Computational Experiments", *Technometrics.*, Vol 32 (2), pp. 161–174, 1991.

[2] F. Campolongo, A. Saltelli, "Design of experiments", in: A. Saltelli, K. Chan, M. Scott (Eds.), *Sensitivity Analysis*, *Probability and Statistics Series*, John Wiley, pp. 5163, 2000.

[3] F Campolongo, J Cariboni, A. Saltelli, "An effective screening design for sensitivity analysis of large models", *Environmental Modelling & Software*, Elsevier, Vol. 22 (10), pp. 1509–1518, 2007.

[4] A. Saltelli, P. Annoni, I. Azzini, F. Campolongo, M. Ratto, S. Tarantola, "Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index", *Comput. Phys. Commun.*, Vol 181, pp. 259–270, 2010.

[5] F. Campolongo, A. Saltelli, J. Cariboni, "From screening to quantitative sensitivity analysis. A unified approach", *Comput. Phys. Commun.*, Vol. 182, pp. 978–988, 2011.

[6] F. Campolongo, R.D. Braddock, "The use of graph theory in the sensitivity analysis of the model output: a second order screening method," *Reliability Engineering and System Safety*, Vol. 64 (1), pp. 1–12, 1999.

[7] R.A. Cropp, R.D. Braddock, "The New Morris Method: an efficient second-order screening method," *Reliability Engineering & System Safety*, Elsevier, Vol 78 (1), pp. 77–83, 2002.

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Estimation of the Sobol indices in a linear functional multidimensional model

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Many mathematical models encountered in applied sciences involve a large number of poorly-known parameters as inputs. It is important for the practitioner to assess the impact of this uncertainty on the model output. An aspect of this assessment is sensitivity analysis, which aims to identify the most sensitive parameters, that is, parameters having the largest influence on the output. In global stochastic sensitivity analysis (see for example [11] and [12] and references therein) the input variables are assumed to be independent random variables. Their probability distributions account for the practitioner's belief about the input uncertainty. This turns the model output into a random variable, whose total variance can be split down into different partial variances (this is the so-called Hoeffding decomposition see [16]). Each of these partial variances measures the uncertainty on the output induced by each input variable uncertainty. By considering the ratio of each partial variance to the total variance, we obtain a measure of importance for each input variable that is called the *Sobol index* or *sensitivity index* of the variable [13]; the most sensitive parameters can then be identified and ranked as the parameters with the largest Sobol indices.

Once the Sobol indices have been defined, the question of their effective computation or estimation remains open. In practice, one has to estimate (in a statistical sense) those indices using a finite sample of evaluations of model outputs [4]. Many Monte Carlo or quasi Monte Carlo approaches have been developed by the experimental sciences and engineering communities. This includes the Fourier Amplitude Sensitivity Test (FAST) methods (see for example [2], [15] and references therein) and the Sobol pick-freeze (SPF) scheme (see [13], [14]). Nevertheless, those methods require many evaluations of model outputs which can be a strong limitation when those evaluations are expensive. Many approaches have been developped to overcome this issue. The most popular are Bayesian approach (see for example [11]) or the construction of metamodels. As mentioned in Kleijnen [7] (see equation (1) page 121) one can use functional linear regression as metamodel. In this paper, we study the particular context of the functional linear regression and propose a new way of estimation. We consider nonparametric estimators of quadratic functionals by projection methods, which are related to the procedures developed by Laurent (see [8], [9]) in a density model and by Da Veiga and Gamboa in [3] in a regression model. This method allows us to estimate simultaneously all the Sobol indices with a single sample of reasonable size.

More precisely we consider a separable Hilbert space $\mathbb{H}$ endowed with the scalar product $<,>$ and $X^1, \ldots, X^p$, p independent centered, $\mathbb{H}$-valued, stochastic processes. The model that we consider is a linear regression model :

$$Y = \mu + \sum_{k=1}^{p} < \beta^k, X^k > + \varepsilon.$$

where $\beta_i, 1 \leq i \leq p$ are elements of $\mathbb{H}$, μ is in $\mathbb{R}$ and ε is a centered noise independent of the processes $X_1, \ldots, X_p$.

Our approach is based on the so-called Karhunen-Loève decomposition of the processes X^k ([10], [1]). Thanks to this decomposition we construct natural estimators of the Sobol indices for which we prove asymptotic normality and efficiency. Asymptotic efficiency is a natural property which generalizes the notion of minimum variance unbiased estimator, see [16] chapters 8 and 25 or [6] for more details. Finally we compare this method with the classical SPF [5] and give numerical illustrations on a benchmark model.

References:

[1] J.C. Bronski, "Small ball constants and tight eigenvalue asymptotics for fractional Brownian motions", *J. Theoret. Probab.*, **16**(1):87–100, 2003.

[2] R.I. Cukier and H.B. Levine and K.E. Shuler, "Nonlinear sensitivity analysis of multiparameter model systems", *Journal of computational physics*, **26**(1):1–42, 1978.

[3] S. Da Veiga and F. Gamboa, "Efficient estimation of Sensitivity Indices", *Journal of Nonparametric Statistics, in press*, http://arxiv.org/abs/1203.2899, 2008.

[4] J.C. Helton and J.D. Johnson and C.J. Sallaberryand C.B. Storlie, "Survey of sampling-based methods for uncertainty and sensitivity analysis", *Reliability Engineering & System Safety*, **91**(10-11):1175–1209, 2006.

[5] F. Gamboa and A. Janon and T. Klein and A. Lagnoux and M. Nodet and C. Prieur, "Statistical inference for Sobol pick freeze Monte Carlo method", *In revision ESAIM Proba. Stat.*, 2012.

[6] I.A. Ibragimov and R.Z. Has' Minskii, "Statistical estimation-asymptotic theory", *Springer*, **16**, 1981.

[7] J.P.C. Kleijnen, "Sensitivity analysis and related analyses: A review of some statistical techniques", *Journal of Statistical Computation and Simulation*, **57**(1-4):111–142, 1997.

[8] B. Laurent, "Efficient estimation of integral functionals of a density", *Ann. Statist.*, **24**(2):659–681, 1996.

[9] B. Laurent, "Adaptive estimation of a quadratic functional of a density by model selection", *ESAIM Probab. Stat.*, **9**:1–18, 2005.

[10] H. Luschgy and G. Pagès, "Functional quantization of Gaussian processes", *J. Funct. Anal.*, **196**(2):486–531, 2002.

[11] J.E. Oakley and A. O'Hagan, "Probabilistic sensitivity analysis of complex models: a Bayesian approach", *J. R. Stat. Soc. Ser. B Stat. Methodol.*, **66**(3):751–769, 2004.

[12] A. Saltelli, "Making best use of model evaluations to compute sensitivity indices", *Computer Physics Communications*, **145**(2):280–297, 2002.

[13] I.M. Sobol, "Sensitivity estimates for nonlinear mathematical models", *Math. Modeling Comput. Experiment*, **1**(4):407–414, 1993.

[14] I.M. Sobol, "Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates", Mathematics and Computers in Simulation, **55**(1-3):271–280, 2001.

[15] J.Y. Tissot and C. Prieur, "A bias correction method for the estimation of sensitivity indices based on random balance designs", *J. Roy. Statist. Soc.*, 2010.

[16] A.W. Van der Vaart, "Asymptotic statistics", *Cambridge Univ Press*, 2000.

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Time-dependent sensitivity and uncertainty analyses of an agro-climatic model for the water status management of vineyard

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This work describes the global sensitivity analysis (SA) of an agro-climatic model embedded in a decision support system (DSS) for the water status management of vineyard in the Languedoc-Roussillon region, France. The DSS is used in real time to recommend irrigation amounts in order to maintain optimal vine water stress dynamics, based on the quality objective targeted by the winegrower (table wine, aging or laying-down wine, etc.). A major characteristic of agro-climatic models is the difficulty of estimating the numerous input parameters because field measurements are both costly and tedious. This is particularly true when soil-related parameters are involved - which is the case here - because their estimation requires subsoil measurements. The operational use of the model thus requires finding the right balance between data-friendliness and precision: the less input parameters asked to the end-user, the better. In this context, in addition to the obvious interest for the modeller in gaining insight into the model behaviour, the practical use of the SA is twofold. It is first to identify the most influent parameters in order either to concentrate experimental efforts on their field measurement when possible, or to calibrate them otherwise. It is then to measure the ouputs uncertainty – computed along with the sensitivity indices – to parameters estimation in order to provide the end-user with confidence indices on the DSS irrigation recommendations. After a preliminary screening of the less influential parameters via Morris method [1], the SA is achieved with Sobol method [2]. The model includes a temporal output and correlated temporal inputs, so the study addresses some issues arising from these two aspects when met in a practical context.

Several model outputs are analyzed. The first one is a discrete-time (daily) output called the predawn leaf water potential (PLWP) that measures in MPa the water status in vine leaves. It is the reference indicator of vine water status, which describes the physiological state that vine experiences under water deficit. It is estimated based on a discrete-time mechanistic soil-vegetation-atmosphere-transfer model [4], i.e. through the combination of models describing the dynamics of soil water balance, vine canopy growth and solar radiation absorbed by the vegetation. The soil water balance model is itself the combination of sub-models describing the various soil water transfer processes: rain and irrigation infiltration, bare soil evaporation, vine root absorption, runoff and drainage. The soil water balance model runs daily starting January 1st, and the PLWP is computed daily during the vine vegetative cycle, i.e. when leaves are present, typically from April till October. The other outputs of interest are scalar outputs related to the DSS irrigation recommandations: triggering date and amount. They are computed when the PLWP falls below an optimal range, defined by the winegrower and varying over time. For a practical use of the model in a DSS, these are the outputs whose uncertainty and sensitivity to inputs variability is the most critical to assess. The model requires the definition of 4 temporal and 22 scalar inputs. The 4 temporal inputs are to some extend correlated. They represent the weather data necessary for driving the model: daily precipitations, solar radiation, mean air temperature and potential evapotranspiration, and are in practice measured by a weather station.

Firstly, the SA was achieved at the Languedoc-Roussillon scale on the temporal PLWP output only, in order to gain a general insight into the model behaviour. The distributions of all scalar

parameters were set rather easily from literature or field expertise in order to scan their whole variation range at the regional scale. The case of the weather data was more an issue, since to the authors' knowledge, the introduction of correlated functional inputs in a SA is still under research. The solution chosen was to use an equivalent of the map-labeling method develop for spatial inputs [4]. It consists in grouping the 4 temporal inputs into a single one, defining a weather scenario. The weather scenarios are then equiprobably drawn among 22 sets of data (i.e. scenarios) collected in various spots of the Languedoc-Roussilon in the past 40 years, and representative of dry, medium-dry and humid years. A preliminary screening via Morris method allowed to identify 6 parameters as being negligible, and consequently to fix them to nominal values. These are the soil albedo, which depicts the radiation reflecting power of the soil surface, and the 5 cumulative thermal times defining the transition between phenological stages (leaf appearance, flowering, etc.). A Sobol SA was then achieved, and the first order and total sensitivity indices were computed sequentially at each simulation step, which enables to follow the variation of parameters influence over time. Results showed the predominant influence of the weather data and of the total transpirable soil water (TTSW) parameter controlling the maximum amount of soil-water available to the vine, which confirms the empirical knowledge of the modelers. Yet one drawback of the method is that it does not allow to quantify the individual influence of the weather components, and especially of precipitations that are empirically known to be the most influent one.

The second step was to quantify at the vine plot scale the sensitivity to inputs estimation error of the PLWP, and most importantly of the irrigation amount and triggering date. Since simulations are rather time-consuming, the regional-scale results were used to help defining 12 vine plots representative of the Languedoc-Roussillon variability and restrict the analysis to them. 3 independent SA (i.e. 36 in total) were then realized for each vine plot for 3 fixed weather scenarios representative of dry, medium-dry and humid years. The aim was thus to test the model sensitivity to the scalar inputs in various fixed pedo-climatic contexts. In all SA, the temporal evolution of the PLWP uncertainty and of the sensitivity indices strongly related to the precipitations histogram, which confirms the critical influence of this weather component. In order to compare the various SA, synthetic sensitivity indices were defined based on previous works [5] to rank parameters according to their global influence on the whole time-dependent simulations. In all cases, the same 3 parameters predominate, even if their relative influence varies from one vine plot to another. These are the TTSW parameter, the soil-water content at January 1st and a soil-water content threshold controlling root absorption. The same 3 parameters have the highest influence on the irrigation recommendations variability, along with the vegetation maximum width. These 3 soil-related parameters, especially the TTSW, are hard to measure and thus hard to directly ask to the end-user. So the suitability of calibrating one or all of them is currently under discussion.

References:

[1] M.D. Morris, "Factorial sampling plans for preliminary computational experiments", *Technometrics*, **33**:161–174, 1991.

[2] I.M. Sobol, "On sensitivity estimation for nonlinear mathematical models.", *Matematicheskoe Modelirovanie*, **2**:112–118, 1990.

[3] E. Lebon, V. Dumas, P. Pieri and H.R. Schultz, "Modelling the seasonal dynamics of the soil water balance of vineyards", *Functional Plant Biology*, **30**:699–710, 2003.

[4] L. Lilburne and S. Tarantola, "Sensitivity analysis of spatial models", *International Journal of Geographical Information Science*, **23**:151–168, 2009.

[5] M.H. Lamboni, H. Monod and D. Makowski, "Multivariate sensitivity analysis to measure global contribution of input factors in dynamic models", *Reliability Engineering and System Safety*, **96**:450–459, 2011.

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Goal-oriented error estimation for reduced basis method Application to certified sensitivity analysis

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The reduced basis method ([2,3]) is a powerful model reduction technique. It is aimed at fast numerical resolution of certain parametrized partial differential equations in a many-query setting, i.e., fast approximation, for a large number of values of μ, of a solution $u(\mu)$ of:

$$\mathcal{L}(\mu, u(\mu)) = f(\mu), \tag{1}$$

where $\mu \in \mathbf{R}^p$ is the parameter vector, $\mathcal{L}(\mu, \cdot)$ is a (discretized) linear differential operator and $f(\mu)$ is a (discretized) function.

We are interested in the approximation of a linear functional ℓ of u: $s(\mu) = \ell(u(\mu))$ by

$$\widetilde{s}(\mu) = \ell(\widetilde{u}(\mu)),$$

where $\widetilde{u}(\mu)$ is the approximate solution of (1) found using the reduced basis method.

More specifically, we want to find an explicitly computable error bound ϵ^s so that:

$$|s(\mu) - \widetilde{s}(\mu)| \leq \epsilon^s(\mu). \tag{2}$$

In [1], we present a numerical algorithm for computing an ϵ^s bound such that (2) holds with great probability.

In this talk, we propose to briefly review the reduced basis method, to present our probabilistic bound $\epsilon^s(\mu)$, to compare it with competing error bounds, and, to finish, to give an application to the certification of a Sobol sensitivity analysis of s (with respect to the components of μ) performed using fast evaluations of its approximation $\widetilde{s}$.

References:

[1] A. Janon, M. Nodet, C. Prieur, "Goal-oriented error estimation for reduced basis method, with application to certified sensitivity analysis", *submitted, available at* `http://hal.inria.fr/hal-00721616`, 2012.

[2] N. C. Nguyen, K. Veroy, A. T. Patera, "Certified Real-Time Solution of Parametrized Partial Differential Equations". In Handbook of Materials Modeling, Springer, 1523–1558, 2005.

[3] C. Prud'homme, D. V. Rovas, K. Veroy, L. Machiels, Y. Maday, A. T. Patera, and G. Turinici, Reliable Real-Time Solution of Parametrized Partial Differential Equations: Reduced-Basis Output Bound Methods. J Fluids Engineering, 124:7080, 2002.

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Application of the control variate technique to the estimation of total sensitivity indices

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There have been many successful improvements in the efficiency of estimating the main effect Sobol' indices ran in from the advanced formulas for small sensitivity indices to application of RBD and various metamodelling methods [1]. However, there have been no similar advances concerning computation of the total sensitivity indices and the Sobol-Jansen formula [2] remains to be the only formula used in the direct computation of the total sensitivity indices. To improve the efficiency of the MC estimates for total sensitivity indices we apply the variance reduction technique and develop a new formula for the evaluation of total sensitivity indices. We also present results using well known test functions.

Consider the integral of the function f over the n-dimensional unit hypercube H^n. For the estimation by the Monte Carlo method, an integration error $\varepsilon_{MC} = \sigma/N^{0.5}$, where σ^2 is the variance of $f(x)$. The control variate method is used to decrease ε_{MC} by reducing σ^2. In the control variate method we define a new integrand $\tilde{f}(x) = f(x) + C\big(g(x) - \mu_g\big)$, where C is a constant coefficient and $g(x)$ is a function for which $\mu_g = \int g(x)dx$ is known. $g(x)$ is called a control variate. The difficulty is to find a good control variate g to build an unbiased estimator $\tilde{f}$ with a reduced variance.

We apply the control variate technique to the evaluation of the total sensitivity indices S_j^T for the case of a single variable x_j. The same approach can be easily generalised for the case of a set of variables. The Sobol- Jansen formula has a form:

$$S_j^T = \frac{1}{2D}\int \left[f(x) - f(x_j', z)\right]^2 dx dx_j' \qquad (1)$$

Consider the ANOVA decomposition:

$$f(x) = f_0 + \sum_{j=1}^{n} f_j(x_j) + \sum_{0\le i<j\le n} f_{ij}(x_i, x_j) + \cdots + f_{i\ldots n}(x_i, \ldots, x_n) \qquad (2)$$

A natural choice for the control variate for a function $f(x)$ is to choose the first order terms $g(x) = f_0 + \sum_{j=1}^{n} f_j(x_j)$ of ANOVA. It leads to the following result:

Theorem: Formula for the evaluation of the total sensitivity indices S_j^T using the control variate (CV) technique has a form

$$S_j^T = \frac{1}{2D}\int \left[f(x) - f_j(x_j) - \left[f(x_j', z) - f_j(x_j')\right]\right]^2 dx dx_j' + S_j \qquad (3)$$

Clearly $Var\left[f(x) - f_j(x_j) - \left[f(x_j', z) - f_j(x_j')\right]\right] \le Var\left[f(x) - f(x_j', z)\right]$ because $2DS_j \ge 0$. Hence formula (3) is more efficient for estimation of S_j^T using the MC method for

Type A and B functions for which S_j^T is close to S_j [3]. However, it requires the knowledge of the first order ANOVA terms $f_j(x_j)$ and the corresponding S_j. In a general case of functions not known analytically $f_j(x_j)$ and S_j can only be found by building metamodels and then extracting the numerical values of the first order sensitivity indices and approximation of the first terms of the ANOVA decomposition from metamodels.

In this project, we approximate the functions $f_j(x_j)$'s by usin the Generalized Additive Models [4] with an identity link function. In this method $f_j(x_j)$'s are estimated as smoothing penalized regression splines. Once $f_j(x_j)$'s are built, $S_j's$ are numerically estimated.

We apply the developed formula (6) for the total sensitivity indices to the Ishigami function with a=7, b=0.1. From the values of the first order and total indices $S_1 = 0.3138, S_2 = 0.4424, S_3 = 0.0$, $S_1^T = 0.5574, S_2^T = 0.4424, S_3^T = 0.24360,$ it is clear that one can expect the formula with using the control variate technique can give an improvement in efficiency for variables 1 and 3. Indeed, the numerical tests confirm this hypothesis. We evaluated total sensitivity indices S_j^T using the original formula (1) and the improved formula (6). We used 1) analytical expressions for $f_j(x_j)$ and S_j's with MC and QMC sampling; 2) expressions for $f_j(x_j)$ and S_j's obtained from a metamodel. Fig. 1 presents results for the convergence of S_j^T, namely by plotting the root mean square error (RMSE) ε versus N (for definition of RMSE see e.g. [3]). It can be seen that the improvements in convergence are from 10-folds for MC to 10^2–folds for QMC when analytical expressions for $f_j(x_j)$ and S_j's are used. There is also some improvements in conver ence when $f_j(x_j)$ and S_j's are estimated from a metamodel. The efficiency of this method can be also increased further by adding higher order terms to the control variate.

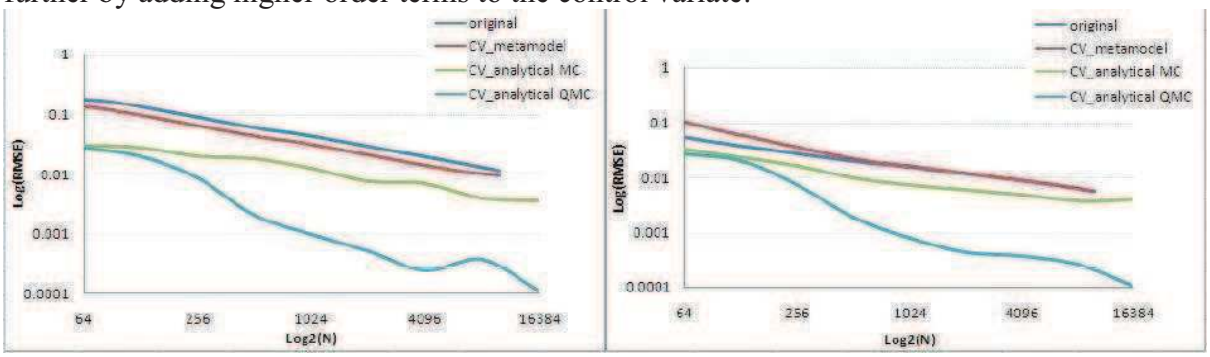

Figure 1: RMS Error vs. N. Variable 1 (left) Variable 2 (right) for the original Sobol Jansen formula (blue line), CV formula based on metamodel (red line), analytical results for $f_j(x_j)$ and S_j using MC (green line), analytical results for $f_j(x_j)$ and S_j using QMC (blue line).

References :

[1] Saltelli A, Annoni P, Azzini I, Campolongo F, Ratto M, Tarantola S. Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index. Computer Physics Communications, **181**(2):259-70, 2010

[2] Sobol' IM. Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. Math Comput Simul, **55**(1–3):271–80, 2001.

[3] Kucherenko S, Feil B, Shah N, Mauntz W. The identification of model effective dimensions using global sensitivity analysis. Reliability Engineering and System Safety 2011;96:440–9.

[4] Hastie, T., Tibshirani, R.: Generalized Additive Models. Chapman and Hall, London, 1990.

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New way of estimating Total Sensitivity Indices

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I. Objective Global Sensitivity Analysis (GSA) methods [1,2] and Multivariate Sensitivity Analysis (MSA) methods [3], which aim to apportion the variability of model output into input variables and their interactions, are an objective way to evaluate the impact of the uncertainty in input variables on the model output. In particular, The Total Sensitivity Index (TSI) gives for each input its overall contribution, including the effects of its interactions with all the other inputs, in the variability of the model output. The computation of TSI requires a large number of model evaluations [1,4]. We investigate a promising way of computing TSI with few model evaluations.

II. Methods Let $Y = f(\mathbf{X})$ be a model output and $\mathbf{X} = (X_1, \ldots, X_d)$, d independent (A1) input factors. Under assumption $\mathbb{E}\left(f^2(\mathbf{X})\right) < +\infty$ (A2) we have the following decompositions:

$$\begin{aligned} f(\mathbf{X}) &= \sum_{u \subset \{1,2,\ldots d\}} f_u(X_u), \qquad [1] \\ &= f_0 + g(X_j, \mathbf{X}_{\sim j}) + h(\mathbf{X}_{\sim j}), \qquad [5] \end{aligned}$$

where, $f_0 = \mathbb{E}\left[f(\mathbf{X})\right]$; $f_j(X_j) = \mathbb{E}\left[f(\mathbf{X})|X_j\right] - f_0$; $\mathbb{E}\left[f_u(X_u)\right] = 0$ and $g(X_j, \mathbf{X}_{\sim j}) = \sum_{u \ni j} f_u(\mathbf{X}_u)$,.

In papers [5] [6], it is shown that the TSI index of X_j is also defined as:

$$S_{T_j} = \frac{\mathbb{E}\left[g^2(X_j, \mathbf{X}_{\sim j})\right]}{\mathbb{V}[f(\mathbf{X})]}. \tag{1}$$

Proposition 1 and Theorem 1 give a practical expression of $g(\cdot)$ and a numerical way of computing $g(\cdot)$ and TSI indices.

Proposition 1: Under assumptions A1 and A2, we have:

$$g(X_j, \mathbf{X}_{\sim j}) = f(\mathbf{X}) - \mathbb{E}\left[f(\mathbf{X})|\mathbf{X}_{\sim j}\right]$$

Proof 1: Due to $f(\mathbf{X}) = f_0 + g(X_j, \mathbf{X}_{\sim j}) + h(\mathbf{X}_{\sim j})$ and $\mathbb{E}\left[g(X_j, \mathbf{X}_{\sim j})|\mathbf{X}_{\sim j}\right] = 0$, we have $\mathbb{E}\left[f(\mathbf{X})|\mathbf{X}_{\sim j}\right] = f_0 + h(\mathbf{X}_{\sim j})$. □

Theorem 1: Let $\mathbf{x}_i$, $i = 1, 2 \ldots, N$ be N realizations of $\mathbf{X}$; $f(\mathbf{X})$, a polynomial of order $2p-1$ with respect to X_j (A3). If A1, A2 A3 hold we have:

i) $g(x_j, \mathbf{x}_{\sim j})$, is exactly known if $\mathbb{E}\left[f(\mathbf{X})|\mathbf{X}_{\sim j} = \mathbf{x}_{\sim j}\right]$ is known
ii) p evaluations of $f(\cdot)$ are sufficient to obtain the exact integral $\mathbb{E}\left[f(\mathbf{X})|\mathbf{X}_{\sim j} = \mathbf{x}_{\sim j}\right]$
iii) $p+1$ evaluations of $f(\cdot)$ are sufficient to obtain the exact value of $g(x_j, \mathbf{x}_{\sim j})$
iv) $\mathbf{N(dp+1)}$ is the total cost of model evaluations to estimate the d TSI indices

Proof 2: i) obvious; ii) Gauss−Legendre quadrature allows an exact computation of $\mathbb{E}\left[f(\mathbf{X})|\mathbf{X}_{\sim j}\right]$ for polynomials of order $2p-1$ with only p evaluations of $f(\cdot)$; iii) and iv) are the consequences of i) and ii). □

Theorem 1 is suitable for polynomial function with respect to each factor. However, it can be used to approximate the TSI indices of any function, bearing in mind the Taylor expansion.

III. Results and Conclusions Theorem 1 is used to estimate the TSI indices of 3 classes of Sobol's function [7] $\left(f(\mathbf{x}) = \prod_{j=1}^{d=10} \frac{|4x_j - 2| + a_j}{1 + a_j}\right)$: Type A, i.e. few important factors; Type B, all factors are important without any interaction; Type C, all factors are important by interaction. Table 1 shows the average of 50 estimations of TSI based on Sobol' sequence design and Figure 1 shows the sum of the d mean absolute errors. Results are interesting for Type A and B functions (best case). For Type C, the estimations vary a little bit after 30000 model evaluations, suggesting

	Type A: $\mathbf{a} = (0, 0, 6.52, \ldots, 6.52)$		Type B: $\mathbf{a} = (50, \ldots, 50)$		Type C: $\mathbf{a} = (0, \ldots, 0)$	
Input	$S_{T.j}$	$\widehat{S_{T.j}}$	$S_{T.j}$	$\widehat{S_{T.j}}$	$S_{T.j}$	$\widehat{S_{T.j}}$
X1	0.54	0.5676	0.1	0.1062	0.27	0.2687
X2	0.54	0.5515	0.1	0.1070	0.27	0.1653
X3	0.013	0.0135	0.1	0.1066	0.27	0.2272
X4	0.013	0.0125	0.1	0.1059	0.27	0.1641
X5	0.013	0.0158	0.1	0.1050	0.27	0.2616
X6	0.013	0.0126	0.1	0.1064	0.27	0.2703
X7	0.013	0.0123	0.1	0.1072	0.27	0.3312
X8	0.013	0.0153	0.1	0.1076	0.27	0.2578
X9	0.013	0.0131	0.1	0.1064	0.27	0.2667
X10	0.013	0.0148	0.1	0.1056	0.27	0.3575
$\mathbf{N(dp+1)}$		**3780**		**3780**		**30380**

Table 1: True TSI indices and average of 50 estimations of TSI indices for Sobol's function

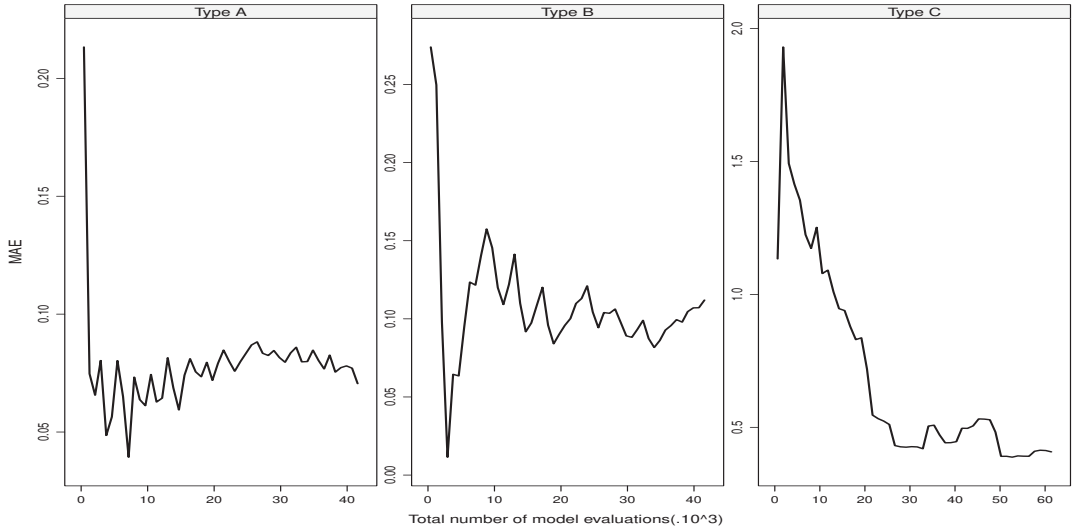

Figure 1: Sum of $d = 10$ mean absolute errors for TSI estimations versus total cost of analysis

a possibility and a need to improve the method rather than increasing the number of model evaluations. However, the results are comparable to those obtained in [4].

References: -[1] I. M. Sobol. Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. Math. and Comp. in Simul 55, pp. 271280, 2001.

-[2] A. Saltelli, M. Ratto, T. Andres, F. Campolongo, J. Cariboni, D. Gatelli, M. Saisana, and S. Tarantola. Global Sensitivity Analysis: the Primer. Wiley, New York, 2008.

-[3] M. Lamboni, H. Monod, and D. Makowski. Multivariate sensitivity analysis to measure global contribution of input factors in dynamic models. RESS, 96, pp. 450-459, 2011.

-[4] A. Saltelli, P. Annoni, I. Azzini, F. Campolongo, M. Ratto and S. Tarantola. Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index. Comp. Phy. Com. 181, pp. 259-270, 2010.

-[5] M. Lamboni, B. Iooss, A.-L. Popelin, F. Gamboa, Derivative-based global sensitivity measures: general links with Sobol' indices and numerical tests, Mathematics and Computers in Simulation, Available online 19/02/2013.

-[6] I.M. Sobol, S. Kucherenko, Derivative based Global Sensitivity Measures and their link with global sensitivity indices, Mathematics and Computers in Simulation, V 79, Issue 10, pp. 3009-3017, June 2009.

-[7] S. Kucherenko, M. Rodriguez-Fernandez, C. Pantelides, N. Shah. Monte Carlo evaluation of derivative based global sensitivity measures. Reliability Engineering System Safety ,Vol. 94, Issue 7, p 1135-1148, 2009.

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Multidimensional Global Sensitivity Analysis for Aircraft Infrared Signature Models with Dependent Inputs

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1. Context

Progress made during the last fifty years in optics sensors enhanced the use of InfraRed (IR) detection for scientific, surveillance and military applications. IR sensors enable to detect targets that cannot be set apart from their surroundings in the visible spectral range, thanks to their emitted heat. This explains why knowledge of aircraft IR emission is compulsory: for example in order to assess their detection probability and thus their susceptibility, and why IR signature (IRS) analysis is important. For many reasons, the experimental approach is generally not feasible to evaluate the IRS, and computer programs are therefore extremely valuable tools.
In the last decade, the usefulness of multispectral or hyperspectral sensors for remote sensing assignments has been proven [1-2], and some studies [3-4] emphasize their potential for target detection. However, few multispectral sensors are, for now, available in the IR field. In this study, we focus on the specification of a multispectral sensor for different missions, such as aircraft detection or classification. ONERA has developed for thirty years a simulation of aircraft IRS, CRIRA, initiated by [5]. Using CRIRA, we aim at performing a sensitivity analysis, to identify inputs that have negligible influence on the computed IRS, and can be set at a constant value.
For an aircraft in a given atmospheric environment, the first order effects on the IRS relate to the spectral range, the presentation geometry, the aircraft speed and the engine power setting. Several sources of variability lead to a dispersion of the values likely to be observed: weather, aircraft aspect angles, aircraft type, optical properties. Some input variables of CRIRA are qualitative: the atmospheric model, the model of aerosol, for example, and quantitative variables related to atmospheric conditions, such as the relative humidity of the atmosphere, the ground's air temperature and the altitude of the cloud layer's base, are correlated.
We consider vectorial outputs: the IRS spectrally integrated in about 5 up to 20 contiguous bands. Moreover, a single run of our simulation requires about three minutes; we thus keep the number of simulation runs below 1000 for the sensitivity analysis. Hence, we have to perform a multidimensional global sensitivity analysis with four constraints:

- a number of simulation runs that must be small (<1000),
- quantitative inputs that are correlated,
- presence of qualitative inputs,
- correlated multidimensional outputs.

2. Methodology

Several approaches enable to carry out the sensitivity analysis of a computer simulation, among which stand out Sobol' Sensitivity Indices (SSI) estimation, described in [6]. Most of the published methods are based on Monte Carlo or Quasi Monte Carlo simulations and require thousands or even tens of thousands of simulation runs for computing accurate estimations of the SSI. Moreover, only a few methods enable to account for dependent quantitative inputs, either by generalizing variance-based sensitivity indices [7-9] or by using distribution-based sensitivity indices [10].
We thus make use of an approach that is jointly based on a Partial Least Squares Regression metamodelling and on a D-Optimal Computer Experiment Design strategy, proposed in [11] and

implemented in R. This methodology enables to compute specific sensitivity indices, referred to as SI-VIP, under our four constraints.
It is based on a small size D-optimal design, formed by computer experiments selected from a large (about 10000 points) correlated network of candidate simulations. In this work, we use copulas [12] for correlating the quantitative inputs, and we assume that the outputs can be approximated by an incomplete polynomial metamodel of degree 3 (the categorical inputs are coded with their (0/1)-indicator variables), with chosen monomials. We make use of an exchange algorithm for the optimization of the normalized determinant of the information matrix associated to this metamodel and we choose the size of the final D-optimal design so as to perform a good compromise between a high level of the D-optimality criterion and a not too large number of simulation runs.
The simulation outputs for all numerical experiments prescribed by the design are then collected, the coefficients of the polynomial metamodel computed by PLS regression, and the sensitivity indices estimated. The SI-VIP indices can reveal the more influent inputs for all the outputs studied simultaneously, which accounts for our fourth constraint and is especially useful when the multivariate output is a (multi)spectral one.

3. Results

Very promising results have been obtained applying the proposed methodology on a test case for a standard air-to-ground detection scenario, namely a daylight air-to-ground full-frontal approach by a generic aircraft flying at low altitude. We were able to identify 10 variables among 26 that have a strong impact on integrated and multispectral IRS variability for the chosen scenario, with only 180 simulations. Being able to perform a sensitivity analysis simultaneously in dozens of spectral bands is especially interesting: we can thereby consider different selections and mergings of bands, and carry through the specification of a multispectral sensor.

References :

[1] L. E. Hoff, A. M. Chen, X. Yu, and E. M. Winter, "Enhanced Classification Performance from Multiband Infrared Imagery ", *IEEE Proceedings of ASILOMAR-29,* 837-841, 1996.
[2] C. I. Chang and S. S. Chiang, "Anomaly detection and Classification for Hyperspectral Imagery ", *IEEE Trans. Geosci. Remote Sensing*, **40**: 1314-1325, 2002.
[3] J. Karlholm and I. Renhorn, “Wavelength band selection method for multispectral target detection”, *Applied Optics*, **41**(32):6786-6795, 2002.
[4] D. Manolakis and G. Shaw, “Detection algorithms for hyperspectral imaging applications”, *IEEE Signal Process. Mag.*, **19**:29-43, 2002.
[5] G. Gauffre, “Aircraft infrared radiation modeling”, *Rech. Aerosp.*, **4**:245–26, 1981.
[6] I.M. Sobol, “Sensitivity estimates for nonlinear mathematical models”, *Mathematical Modelling and Computational Experiments*, **1**:407-414, 1993.
[7] T.A. Mara, S. Tarantola, “Variance-based sensitivity indices for models with dependent inputs”, *Reliability Engineering and System Safety,* **107**:115-121, 2012.
[8] S. Kucherenko, S. Tarantola, P. Annoni, “Estimation of global sensitivity indices for models with dependent variables”, Computer Physics Communications, **183**: 937–946, 2012.
[9] G. Chastaing, F. Gamboa, C. Prieur, “Generalized Hoeffding-Sobol Decomposition for Dependent Variables -Application to Sensitivity Analysis”, http://arxiv.org/abs/1112.1788v3.
[10] E. Borgonovo, S. Tarantola, “Moment Independent and Variance-Based Sensitivity Analysis with Correlations: An Application to the Stability of a Chemical Reactor”, Int. J. of Chemical Kinetics **40**(11): 687-698, 2008.
[11] J.P. Gauchi, S. Lehuta and S. Mahévas, "Optimal Sensitivity Analysis under Constraints: Application to Fisheries," *Procedia Social and Behavioral Sciences*, **2**:7658-7659, 2010.
[12] R. B. Nelsen, “An Introduction to Copula” 2nd Ed., Springer, 2006.

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Multi-fidelity sensitivity analysis

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Complex computer models, used in science and engineering to model physical phenomena, frequently have a large number of input parameters. To finely analyse these codes, the determination of the important input parameters can be carried out by a global sensitivity analysis. We focus on Sobol indices [6] which are a variance-based importance measures of model input parameters on a model response. Nevertheless, the estimation of the Sobol indices by sampling methods requires large number of simulations, that are sometimes too costly and time-consuming. A well known method to overcome this difficulty is to build a mathematical approximation of the code output - also called surrogate model or metamodel - from a limited number of simulations of the real code. A very popular class of surrogate models is the Gaussian process regression, also called kriging.

The goal of this paper is to take advantage of the property that a computer code can often be run at different levels of accuracy. In this case, the so-called multi-fidelity co-kriging surrogate modeling [2] can be used to predict the output of the complex computer code and thus to perform a global sensitivity analysis. For this purpose, we introduce non-asymptotics certified multi-fidelity Sobol indices, i.e. with confidence intervals which take into account the surrogate model error when the number of simulations is small.

Let $y(x)$ be the scalar output of a complex code and $y_1(x)$ be a less accurate and faster version of this code. The idea is to suppose that the prior knowledge about the response of codes can be modeled by Gaussian processes. The multi-fidelity cokriging model [2] is defined as the following auto-regressive model :

$$Y(x) = \rho Y_1(x) + \delta(x) \tag{1}$$

where $\delta(x) \sim \mathrm{GP}(\mathbf{f}_\delta'(x)\beta_\delta, \sigma_\delta^2 r_\delta(x,x'))$, $Y_1(x) \sim \mathrm{GP}(\mathbf{f}_1'(x)\beta_1, \sigma_1^2 r_1(x,x'))$ and $Y_1(x)$ is independent of $\delta(x)$. The surrogate model is given by the distribution of the Gaussian process $Y(x)$ conditioned by the known values of $y(.)$ and $y_1(.)$ at points in $\mathbf{D} = \{x^{(1)}, \ldots, x^{(N)}\}$ and $\mathbf{D}_1 = \{x^{(1)}, \ldots, x^{(N)}, x^{(N+1)}, \ldots, x^{(N_1)}\}$. We use the notations $\mathbf{y} = y(\mathbf{D})$, $\mathbf{y}_1 = y_1(\mathbf{D}_1)$, $\mathbf{Y} = Y(\mathbf{D})$ and $\mathbf{Y}_1 = Y_1(\mathbf{D}_1)$. The mean and the covariance of the conditional distribution of $Y(.)$ given $\mathbf{Y} = \mathbf{y}, \mathbf{Y}_1 = \mathbf{y}_1$ have the following form [3]:

$$\mathbb{E}[Y(x)|\mathbf{Y} = \mathbf{y}, \mathbf{Y}_1 = \mathbf{y}_1] = \hat{\rho}\mu_1(x) + \mu_\delta(x) \tag{2}$$

$$\mathrm{cov}(Y(x), Y(\tilde{x})|\mathbf{Y} = \mathbf{y}, \mathbf{Y}_1 = \mathbf{y}_1) = \hat{\rho}^2 s_1^2(x,\tilde{x}) + s_\delta^2(x,\tilde{x}) \tag{3}$$

The important property is that $\hat{\rho}^2 s_1^2(x,\tilde{x})$ and $s_\delta^2(x,\tilde{x})$ represent respectively the contribution of the coarse code to the total variance and the contribution of the model error between the complex code and the coarse code to the total variance.

Let us suppose that the input parameters $X = (X^1, X^2)$ are independent random variables $X^1 \in \mathbb{R}^{p_1}$ and $X^2 \in \mathbb{R}^{p_2}$. We are interested in the following Sobol index [6]:

$$S^{X_1} = \frac{\mathrm{var}\left(\mathbf{E}\left[y(X)|X^1\right]\right)}{\mathrm{var}\left(y(X)\right)} = \frac{V^{X^1}}{V}, \tag{4}$$

where $\mathbf{E}$ is the expectation with respect to the distribution of the input parameters X.

When we replace the true function by its multi-fidelity approximation, a first estimator for V^{X^1} can be proposed :

$$\begin{aligned} V_{N,N_1,n}^{X^1} &= \frac{1}{n}\sum_{i=1}^{n} Y_{N,N_1}(x_i^1, x_i^2) Y_{N,N_1}(x_i^1, \tilde{x}_i^2) \\ &\quad -\frac{1}{n}\sum_{i=1}^{n} Y_{N,N_1}(x_i^1, x_i^2) \frac{1}{n}\sum_{i=1}^{n} Y_{N,N_1}(x_i^1, \tilde{x}_i^2), \end{aligned} \tag{5}$$

where $Y_{N,N_1}(x_i^1, x_i^2)$ and $Y_{N,N_1}(x_i^1, \tilde{x}_i^2)$ respectly have the conditional distribution of $Y(.)$ given $\mathbf{Y} = \mathbf{y}, \mathbf{Y}_1 = \mathbf{y}_1$, $(\mathbf{X}_1, \mathbf{X}_2) = [(x_i^1, x_i^2)]_{i=1,\dots,n}$ and $(\mathbf{X}_1, \tilde{\mathbf{X}}_2) = [(x_i^1, \tilde{x}_i^2)]_{i=1,\dots,n}$ with $\mathbf{X}_2$ independent of $\tilde{\mathbf{X}}_2$. We thus have an estimator $V_{N,N_1,n}^{X^1}$ which is a random variable. We note that we can use other estimators of Sobol indices as the the efficient one suggested in [1]. We denote by $V_{N,N_1,n}$ the corresponding estimator of V.

We hence can define a first Gaussian process-based multi-fidelity sensitivity index (it corresponds to the one suggested in [4] and [5] in a kriging framework) by the ratio between the expected value of $V_{N,N_1,n}^{X^1}$ and the expected value of $V_{N,N_1,n}$ thanks to the equations (2) and (3). The first advantage of the proposed method is that we have a closed form expression for the two expectations without processing numerical integrations. The second advantage is that we can evaluate the contribution of the coarse code, the bias between the two codes and the covariance between the bias and the coarse code with respect to the distribution of the input parameters.

The main flaw in the previous multi-fidelity sensitivity index is that we considered the variance of the main effects and the total variance separately. Therefore, we propose a second Gaussian process-based multi-fidelity sensitivity index. It is defined as the expected value of the ratio between $V_{N,N_1,n}^{X^1}$ and $V_{N,N_1,n}$. Nevertheless, we cannot obtain closed form expressions for the mean or the variance of this index. A numerical estimation will consist in sampling m realizations of the random vectors $Y_{N,N_1}(\mathbf{X}_1, \mathbf{X}_2)$ and $Y_{N,N_1}(\mathbf{X}_1, \tilde{\mathbf{X}}_2)$ and computing $V_{N,N_1,n}^{X^1}/V_{N,N_1,n}$ for each realization.

However, computing such realizations could lead to numerical issues such as ill-conditioning or huge computational cost (especially if we use a Cholesky's decomposition). To avoid those difficulties, we express the conditioned Gaussian processes included into the model as a linear transformation of non-conditioned stationary Gaussian processes. Then we sample them using the Karhunen-Loeve decomposition of the non-conditioned stationary Gaussian processes.

Sampling with respect to the distribution of $Y_{N,N_1}(\mathbf{X}_1, \mathbf{X}_2)$ and $Y_{N,N_1}(\mathbf{X}_1, \tilde{\mathbf{X}}_2)$ in order to obtain the distribution of $V_{N,N_1,n}^{X^1}/V_{N,N_1,n}$ could be an issue since the conditional distribution $Y(.)$ given $\mathbf{Y} = \mathbf{y}, \mathbf{Y}_1 = \mathbf{y}_1$ is not Gaussian. We note that the non-normality is due to the product of the two Gaussian random variables ρ and $Y_1(x)$. We propose a method to tackle this issue.

These two Gaussian process-based multi-fidelity sensitivity indices are finally illustrated on toy examples and applied to a mechanical problem.

References:

[1] A. Janon, T. Klein, A. Lagnoux, M. Nodet and C. Prieur "Asymptotic normality and efficiency of two Sobol index estimators", submitted, 2012.

[2] M.C. Kennedy and A O'Hagan, "Predicting the output from a complex computer code when fast approximations are available", *Biometrika*, **87**:1–13, 2000.

[3] L. Le Gratiet, "Recursive co-kriging model for design of computer experiments with multiple levels of fidelity with an application to hydrodynamic", submitted, 2012.

[4] A. Marrel, B. Iooss, B. Laurent and O. Roustant, "Calculations of Sobol indices for the gaussian process metamodel", *Reliability Engineering and System Safety*, **94**:742–751, 2009.

[5] J.E. Oakley and A O'Hagan, "Probabilistic sensitivity analysis of complex models: A bayesian approach", *Journal of the Royal Statistical Society*, **B66**(3):751–769, 2004.

[6] I. Sobol, "Sensitivity estimates for non linear mathematical models". *Mathematical Modelling and Computational Experiments*, **1**:407:414, 1993.

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A new class of covariance kernels accounting for non-additivity in high-dimensional kriging

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Kriging has been successfully used for approximating multidimensional functions based on a limited number of evaluations, with numerous applications in sensitivity analysis [1]. A known limitation of the approach, however, is the loss in predictability of usual kriging models when the problem dimensionality increases. Inspired by generalized additive models, kriging models with additive kernels have recently been proposed in the literature. They proved beneficial since centered Gaussian processes (GPs) with an additive kernel have additive paths [2].

A central property of additive kriging models is that they rely on a hypothesis of additivity for the underlying function while offering the convenient framework of kriging, with the interpolation property in the case of noiseless evaluations, and a prediction variance enabling to quantify the precision of kriging predictions. However, when using an additive kernel, the covariance matrix of observations may not be invertible, e.g., when evaluations on a grid induce linear dependencies. An option is to add a positive number to the diagonal entries of the covariance matrix as in [2], but this amounts at considering the non-additive part of the function as noise.

Here we propose a novel approach for extending additive kriging models and enable them to properly deal with the non-additive part of the objective function. Our approach is based on complementing the additive kernel with a kernel whose associated GP paths are orthogonal to additive functions (henceforth called ortho-additive). Derivations are conducted in the framework of Hilbert space decompositions (such as, but not limited to the celebrated Sobol' decomposition), and on recent generalizations of them to kernels [3]. In the context of the Sobol' decomposition for a d-dimensional setting this leads to a decomposition of a kernel $k(x, y)$ into 2^{2d} components. Each component describes the contribution of a selection of subsets of the x and y variables to the covariance. We may sketch this decomposition in a $2^d \times 2^d$ matrix where the first $d + 1$ columns and rows correspond to selections of at most one coordinate of x or y, respectively.

Figure 1 shows this matrix for various modeling choices in which the components used are marked in dark colors. The models differ from each other in the extent to which (cross-covariance) effects can be expressed and in the number of required parameters. In the newly proposed model d) we enrich the additive model with an extra ortho-additive component. Doing so the model may require more samples to be accurately trained, but we gain the ability of capturing non-additive effects at the lowest cost, namely by adding just one more model parameter.

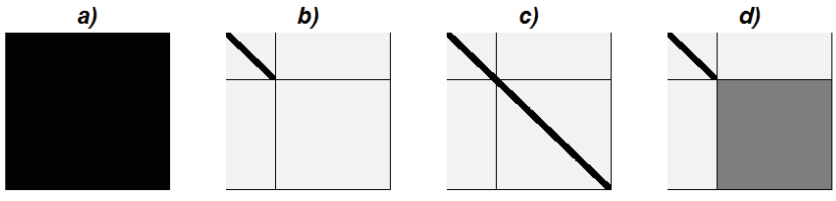

Figure 1: Schematic representation of kernel decompositions; a) full or non-sparse (e.g., Gaussian), b) additive kernels proposed in [2], c) kernels corresponding to processes with uncorrelated Sobol' decomposition terms, d) additive kernels complemented with an ortho-additive kernel.

We consider the Gaussian kernel $k(x, y) = \sigma^2 \cdot e^{-(\frac{\|x-y\|}{\theta})^2}$, which is used in various applications of kriging. By projecting k twice (w.r.t. x and y) onto the orthocomplement of additive functions, we obtain a non-stationary kernel whose associated GP paths are orthogonal to additive functions. E.g., for d=2, we obtain the projected kernel explicitly using the Gaussian error function erf, as

$$\pi_{OA}(k)(x,y) = \sigma^2 \cdot \left(e^{-(\frac{x_1-y_1}{\theta})^2} - E(x_1) - E(y_1) + \mathcal{E}\right)\left(e^{-(\frac{x_2-y_2}{\theta})^2} - E(x_2) - E(y_2) + \mathcal{E}\right) \quad (1)$$

$$\text{with } E(x) = \frac{\sqrt{\pi}\,\theta}{2} \cdot \left(\operatorname{erf}\left(\frac{1-x}{\theta}\right) + \operatorname{erf}\left(\frac{x}{\theta}\right)\right) \text{ and } \mathcal{E} = \sqrt{\pi}\,\theta\,\operatorname{erf}\left(\frac{1}{\theta}\right) + \theta^2\left(e^{\frac{-1}{\theta^2}} - 1\right)$$

Adding an ortho-additive kernel like the one defined in Eq. (1) to additive kernels enables one to create GPs whose covariance structure corresponds to panel d) of Fig. 1. Realizations of such a GP and its split-up into additive and ortho-additive parts are shown in Fig. 2. As illustrated in the last column, this GP is very flexible, even though its kernel is sparser than the Gaussian one.

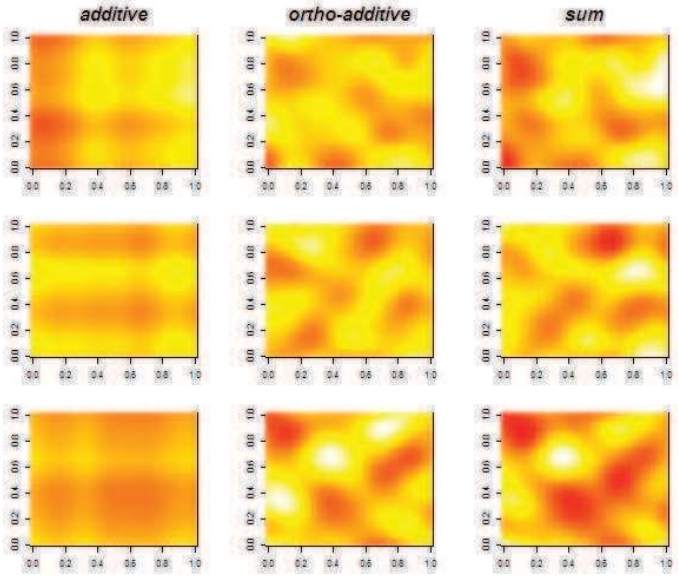

Figure 2: Realizations of GPs; first column: additive part, second column: ortho-additive part; third column: sum of the two, which may be seen as realizations from our new class of GPs.

We demonstrate the potential of the new model in the context of kriging and sensitivity analysis. Introducing a weight parameter for the ortho-additive part allows us to tune but also potentially estimate the degree of additivity. We apply our model to various test cases, and also study the ability of kriging with the proposed class of kernels to approximate realizations of a GP from the corresponding class, depending on several factors such as the degree of additivity, the dimension and the design of experiments.

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References:

[1] J.E. Oakley and A. O'Hagan, "Probabilistic Sensitivity Analysis of Complex Models: A Bayesian Approach", *J. Roy. Statist. Soc.*, **B66**(3):751–769, 2004.

[2] N. Durrande, D. Ginsbourger and O. Roustant, "Additive covariance kernels for high-dimensional Gaussian process modeling", *Ann. Fac. Sci. Toulouse*, **21**(3):481-499, 2012.

[3] D. Ginsbourger, O. Roustant, and N. Durrande, "Covariance-driven invariances of random fields paths", *in preparation.*

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Usefullness of Sensitivity Analysis for Approximate Bayesian Computation

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A first step in the analysis of a parametric statistical model involves the likelihood function. Some models, however, are too complicated for the likelihood to be available in a useful form. Approximate Bayesian Computation (ABC) [1] belongs to a family of likelihood-free Bayesian inference algorithms that attempt to estimate posterior density of parameters where likelihood are intractable. Where θ is the model parameter, posterior density for θ given data D_0 from an observation is given by

$$p(\theta|D_0) \propto f(D_0|\theta)\,\pi(\theta)$$

where $f(D_0|\theta)$ is the likelihood and $\pi(.)$ is the prior density for the parameters. ABC algorithm consists in proposing parameter values and only accepting parameters for which the model generates data that satisfies a performance criteria with respect to the observed data D_0. More precisely, a parameter is accepted if the condition $d(S(D), S(D_0)) \leq \epsilon$ is verified where $d(.,.)$ is a distance, $S(.) = (S_1(.), ..., S_p(.))$ a set of p summary statistics and ϵ defines a policy tolerance for the accepted parameters. This algorithm is an ABC that makes use of the approximation

$$p(\theta|D_0) \approx p(\theta \,|\, d(S(D), S(D_0)) \leq \epsilon).$$

This approximation becomes exact if S is sufficient and $S(D_0) = S(D)$, that is $\epsilon = 0$. Several issues arise with these summary-based methods: curse of dimensionality when using a large number of statistics, use of MCMC approaches to estimate posterior densities and selection of summary statistics.

In this work, we propose to use Sensitivity Analysis (SA) in two ways for parameter estimations with ABC. The first one consists in determining informative statistics $S_j(.)$. In the second one, we propose to use weighted statistics in the definition of distance $d(.,.)$ to improve performance of ABC, when compared to unweighted distance. The weighted distance is defined by

$$d(S(D), S(D_0) = \sum_{j=1}^{p} w_j \left(S_j(D) - S_j(D_0)\right)^2$$

with the constraint on the positive weights $\sum_{j=1}^{p} w_j = 1$. To do this, a criterion is defined to quantify the effects of weights w_j on precision of θ estimates. SA is then used to explore the weight space through a fractional design and we also try to choose optimal weights.

The approach is illustrated with a stochastic architectural model of root systems [2]. This model was designed to integrate the major developmental processes in the simplest way, while using a reduced number of parameters. In our application, θ is a vector of 4 parameters. The number of statistics has been fixed to $p = 15$. These statistics correspond to different analysis on images simulated by the root system model.

References:

[1] M.A. Beaumont, W. Zhang and D.J. Balding, "Approximate Bayesian Computation in Population Genetics", *Genetics*, **162**:2025-2035, 2002.

[2] L. Pagès, "Links between root developmental traits and foraging performance", *Plant, Cell & Environment*, 2011.

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Bayesian quantification of thermodynamic uncertainties in dense gas flows

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Numerical simulations of dense gas flows, i.e. flows of molecularly complex gases at pressures and densities of the general order of magnitude of those of the liquid/vapor critical point, can be extremely sensitive to the model used to describe the fluid thermodynamic behavior [1]. This sensitivity is particularly large for the so-called Bethe–Zeldovich–Thompson (BZT) fluids, which are theoretically predicted to exhibit non-classical gas dynamic behaviors, like expansion discontinuities and splitting shocks, in a tiny thermodynamic region close to the liquid/vapor coexistence curve [2]. Dense gases are encountered in several engineering applications like energy conversion cycles, high-Reynolds wind tunnels, and chemical transport and processing, and are represented by heavy gases with complex molecules, like heavy hydro- and fluorocarbons and siloxanes, for which accurate and comprehensive thermodynamic data are rarely available. As a consequence, high-accurate equations of state (EOS), i.e. thermodynamic laws designed to describe the fluid thermal and caloric behavior in the region of interest, are scarcely found for this class of fluids. Now, reliable simulations of compressible flows with complex thermodynamic behavior require the quantification of thermodynamic modelling errors, especially for those applications that look for improvements of the order of a few percents of the system performance, e.g. energy conversion cycles [3].

For a given EOS, two kinds of uncertainties are encountered. On the one hand, an uncertainty exists on the mathematical form of the EOS to be used for a given fluid; on the other hand, the material-dependent coefficients associated to the equation are imperfectly known. Modelling uncertainties can be reduced to levels on the same order of the experimental uncertainty for molecularly simple well known fluids like water, hydrogen, or carbon dioxide (see [4]), i.e. even as low as 0.1 %. For molecularly complex fluids reserved essentially to an industrial use, like the dense gases of interest here, high accurate experimental data are more hardly available, so that a significant uncertainty on the closure coefficients may exist. Moreover, previous work [1] shows that for some particularly complex gases the model-form uncertainty can be even overwhelming with respect to the parametric uncertainty.

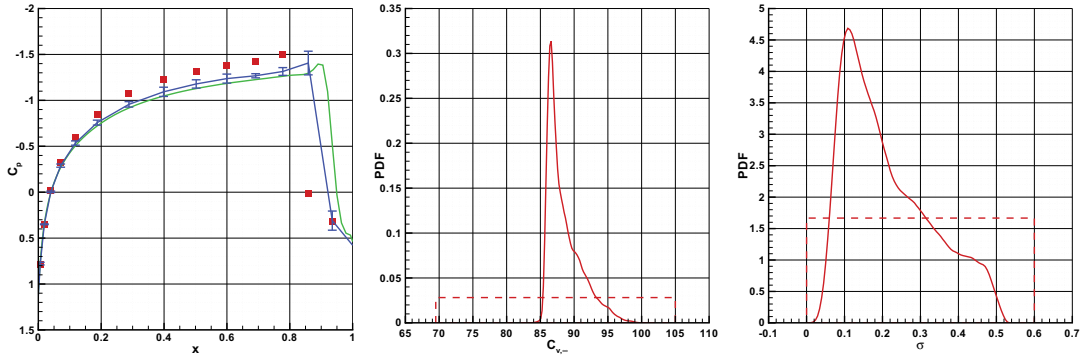
In this work, we adopt a Bayesian approach to quantify modelling uncertainty associated to termodynamic models used for dense gas flow simulations, and investigate the possibility of calibrating thermodynamic models by using aerodynamic data on the flow behavior, instead of strictly thermodynamic information. The statistical model adopted is similar to that used in [5] to calibrate turbulence models for a boundary layer flow.

To this purpose we consider a transonic flow of a silicon oil, namely cyclopentasiloxane (D5), past an airfoil, as in [1]. Numerical solutions of the flow equations are generated by means of a finite volume code based on a third-order accurate numerical scheme [6]. The fluid thermodynamic behavior is modelled using two cubic EOS, namely the Peng-Robinson-Stryjek-Vera [7] (PRSV) and the Soave-Redlich-Kwong [8] (RKS), and a five-term virial EOS, namely the Martin-Hou model [9] (MAH). Without experimental data, calibration data are generated by computing the pressure distribution around the airfoil using a reference EOS based on Helmholtz free energy [10]. The uncertainty on calibration data is estimated to be about 10%. A zero mean Gaussian distribution is used to represent the experimental uncertainty. Pressure data provided by the flow solver for a given choice of the EOS are corrected by using a multiplicative term that accounts for model-form uncertainty. Modelling errors on pressure values computed at different points in the flow field are assumed to be correlated over some distance. The variance of model-form uncertainty term and the correlation length are treated as hyper-parameters and are calibrated from available data along with the EOS closure coefficients.

Markov-chain Monte Carlo sampling of the likelihood function is generated using the Metropolis-Hastings algorithm. Since the numerical dense gas flow model is too expensive to be used in a Monte Carlo algorithm, an approximate model was generated by second-order Lagrange polynomial reconstruction from 3^n samples (n being the number of uncertain coefficients comprised between 3

and 6 according to the EOS considered) of the flow field obtained by running the dense gas solver.

Preliminary results obtained for the PRSV are shown in Fig. 1: (a) represents both the experimental pressure coefficient C_p (red square) along the airfoil wall and the *a priori* output model (green solid line) along with the updated model output (blue solid line, with error bars corresponding to $\pm 3\sigma$); (b) and (c) are prior (dashed) and posterior (solid) pdf for the $C_{v,\infty}$ parameter and the σ hyperparameter.



(a) Values of C_p for data, *a priori* and updated model outputs.

(b) $C_{v,\infty}$'s PDF : prior and posterior.

(c) σ's PDF : prior and posterior.

Figure 1: Preliminary results.

We can observe that the model parameters are well informed, and the updated model output is closer to the data than the prior one, although not completely superposed since the simple cubic PRSV EOS exhibits a large model-form error, on the order of 15% (see Fig. 1-(c)).

At the conference, we will provide a full description of both the numerical and statistical model, along with calibration results for different EOS. Posterior model plausibilities will be used to compare the different EOS and to conclude on the importance of dealing with model-form uncertainty for reliable numerical simulations of dense gas flows.

References:

[1] P. Cinnella *et al.*, "Sensitivity analysis of dense gaz flow simulations to thermodynamic uncertainties", *Phys. Fluids*, **23**: 116101-20, 2011.
[2] M.S. Cramer and A. Kluwick, "On the propagation of waves exhibiting both positive and negative nonlinearity", *J. Fluid Mech.*, **142**: pp 9-37, 1984.
[3] B. Brown and B. Argrow, "Application of Bethe-Zeldovich-Thompson fluids in organic Rankine cycle engines", *J. Propul. Power* , **16** (6): 1118-28, 2000.
[4] R. Span and W. Wagner, "Equations of state for technical applications. I. Simultaneously optimized functional forms for non polar and polar fluids", *Int. J. Thermophys.* , **24**: 1, 2003.
[5] S. H. Cheung *et al.*, "Bayesian uncertainty analysis with applications to turbulence modeling", *Reliability Engineering and System Safety* , **96**: pp 1137-1149, 2011.
[6] P. Cinnella, P. Congedo,"Numerical solver for dense gas flows",*AIAA J.*,**43**: 11 pp 2458-2460, 2005.
[7] R. Stryjek and J. H. Vera, "An improved Peng-Robinson equation of state for pure compounds and mixtures", *Can. J. Chem. Eng.*, **64**: 323, 1986.
[8] G. Soave, "Equilibrium constants from a modified Redlich-Kwong equation of state", *Chem. Eng. Sci.*, **27**: 1197, 1972.
[9] J. J. Martin, Y. C. Hou, "Development of an equation of state for gases", *AIChE J.*, **1**: 142, 1955.
[10] P. Colonna *et al.*, "Multiparameter equations of state for siloxanes: $[(CH3)3-Si-O1/2]_2-[O-Si-(CH3)2]_{i=1,...,3}$ and $[O-Si-(CH3)2]_6$", *Fluid Phase Equilib.*, **263**: 115, 2008.

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Efficient Prediction Designs for Random Fields

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For estimation and prediction of random fields it is increasingly acknowledged that the kriging variance may be a poor representative of the true uncertainty. Experimental designs based on the more elaborate criteria that are appropriate for empirical kriging are very costly to determine. We investigate the possibility of using a compound criteria inspired by an equivalence theorem type relation cf.[1], to build designs sub-optimal for the empirical kriging variance.

The model underlying our investigations is the correlated scalar random field given by

$$Y(x) = \eta(x, \beta) + \varepsilon(x)\,.$$

Here, β is an unknown vector of parameters in R^p, $\eta(\cdot,\cdot)$ a known function and the random term $\varepsilon(x)$ has zero mean, (unknown) variance σ^2 and a parameterized spatial error correlation structure such that $E[\varepsilon(x)\,\varepsilon(x')] = \sigma^2 c(x, x'; \nu)$ with ν some unknown parameters.

We are interested in making predictions $\hat{Y}(\cdot)$ of $Y(\cdot)$ at unsampled locations x in a compact subset X of R^d using observations $Y(x_1), \ldots, Y(x_n)$ collected at a set of design points $\xi = (x_1, \ldots, x_n) \subset X^n$. Our objective is to select ξ (of given size n) in order to maximize the precision of the predictions $\hat{Y}(x)$ over X. One penalized design criterion for such designs is the corrected kriging variance:

$$MEK(\xi) = \max_{x \in X} \left\{ \mathrm{Var}[\hat{Y}(x)] + \mathrm{tr}\left\{ V_\nu \, \mathrm{Var}[\partial \hat{Y}(x)/\partial \nu] \right\} \right\}, \tag{1}$$

with V_ν the covariance of the ML estimator of the covariance parameters ν. Designs ξ that minimize this criterion are called EK(empirical kriging)-optimal. EK-optimal designs are typically not space-filling. This is particularly true for small numbers of observations, when prediction precision is the most sensitive to the detailed geometry of the design. Unfortunately, straightforward maximization of the EK-criterion is computationally demanding. In [4] the use of a convex composition of the two D-optimality criteria for the parameters β and ν is suggested as a surrogate for EK:

$$J_\alpha(\xi) = \alpha \log |M_\beta(\xi, \theta)| + (1 - \alpha) \log |V_\nu^{-1}(\xi, \nu)|, \qquad \alpha \in [0.1]\,, \tag{2}$$

where

$$\begin{pmatrix} M_\beta(\xi,\theta) & 0 \\ 0 & M_\theta(\xi,\theta) \end{pmatrix} = E \left\{ \begin{array}{cc} -\frac{\partial^2 \log L(\beta,\theta)}{\partial\beta\partial\beta'} & -\frac{\partial^2 \log L(\beta,\theta)}{\partial\beta\partial\theta'} \\ -\frac{\partial^2 \log L(\beta,\theta)}{\partial\theta\partial\beta'} & -\frac{\partial^2 \log L(\beta,\theta)}{\partial\theta\partial\theta'} \end{array} \right\},$$

with $L(\beta, \theta)$ the likelihood of β and $\theta = (\sigma^2, \nu)$, and $V_\nu(\xi, \nu)$ in the second term of (2) is the lower diagonal block of $M_\theta^{-1}(\xi, \theta)$.

Although, as it has been shown in [3], a strict equivalence between (1) and (2) does not hold, there is experimental evidence that that optimal designs for one of the criteria tend to perform well under the other, confirming the intuition that finding designs ξ that minimize the EK criterion (1) should be intimately related to finding designs that optimize a suitable combination of the D-optimality criteria for β and ν.

However, the ability to define a constructive experimental design method based on $J_\alpha(\cdot)$ is hampered by the lack of an efficient methodology to select α. In this paper we overcome this difficulty by considering simultaneous optimization of the two criteria $\log |M_\beta(\xi, \theta)|$ and $\log |V_\nu^{-1}(\xi, \nu)|$, and

constraining the candidate set Ξ for the minimization of (1) to the set of non-dominated designs for the corresponding multi-criteria optimization problem. The EK criterion (1) will thus play the role of a preference function for choosing designs in the reduced candidate set Ξ.

Other authors have addressed the determination of experimental designs that simultaneously optimize multiple criteria, constraining the set of possible solutions to the corresponding Pareto surface, *e.g.* [2] where the author discusses the advantages of explicit consideration of the individual criteria over the use of scalar "desirability functions" and proposes several methods to chose amongst the efficient solutions of the Pareto surface. The precise contribution of our work is to use the set of non-dominated solutions of the two identified D-optimality criteria, $\log|M_\beta(\xi,\theta)|$ and $\log|V_\nu^{-1}(\xi,\nu)|$, as a relevant (small) candidate set for EK-optimal designs. We call the designs of this constrained candidate set Pareto-optimal.

For simultaneous optimization of two criteria the Pareto surface reduces to a bounded curve (or to a finite subset of a curve when X is finite). Since the Pareto surface is also the set of maxima of all scalar functions monotone in each criterion, we can construct a finite set of candidate designs by optimizing the compound criterion $J_\alpha(\cdot)$ for a finite set of values of α. Evaluation of the corrected kriging variance over this finite subset allows the determination of a good approximation to the EK-optimal design. As the examples presented will demonstrate, our Pareto-optimal designs have high EK-efficiency, especially for designs with small size n.

References:

[1] J. Kiefer and J. Wolfowitz, "The equivalence of two extremum problems", *Canadian Journal of Mathematics*, **12**:363–366, 1960.

[2] L. Lu, C.M. Anderson-Cook and T.J. Robinson, "Optimization of Designed Experiments Based on Multiple Criteria Utilizing a Pareto Frontier", *Technometrics*, **53**(4):353–365, 2011.

[3] W.G. Müller, L. Pronzato and H. Waldl, "Relations Between Designs for Prediction and Estimation in Random Fields: An Illustrative Case", in E. Porcu, J.-M. Montero and M. Schlather (eds), *Advances and Challenges in Space-time Modelling of Natural Events*, Lecture Notes in Statistics **207**:125–139, 2012.

[4] W.G. Müller and M. Stehlík, "Compound optimal spatial designs", *Environmetrics*, **21**(3-4):354–364, 2010.

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Low cost bounds and estimates of total sensitivity indices based on metamodels

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Model based simulation of complex processes is an efficient approach of exploring and studying systems whose experimental analysis is costly or time-consuming. Good modelling practice requires sensitivity analysis to ensure the model quality by analysing the model structure, selecting the best type of model and effectively identifying the important model parameters. Among the large amount of methods available for the previous purpose, the Global Sensitivity Analysis (GSA) is one of the most efficient and popular ones. GSA methods evaluate the effect of a factor while all the other factors also vary and thus they account for interactions between variables and do not depend on the choice of a nominal point like the local sensitivity analysis methods. Reviews of different global SA methods can be found e.g. in [1]. Variance-based methods, in particular the method of global sensitivity indices (SI) developed originally by Sobol, are one of the most efficient and popular GSA techniques. However, these methods generally require a large number of function evaluations to achieve reasonable convergence and can become impractical for large engineering problems. There are a few efficient techniques for calculating first order Sobol SI. [2] developed the random balance design (RBD) method which is a modification FAST method. In RBD the input space is explored by using one single frequency: this has the advantage of making the computational cost independent from the number of model inputs. Therefore, RBD remains computationally cheap even for models with many inputs. The method is relatively easy to implement, however it only allows the calculation of the first order effects. One of the very important and promising developments of model analysis is the replacement of complex models and models which need to be run repeatedly on-line with equivalent operational metamodels. Several metamodels can be used: polynomials, Gaussian process metamodels [3,4], local polynomials [5], High Dimensional Model Representation (HDMR) based on polynomial chaos expansion [6,7,8]. A practical form of HDMR, Random Sampling-HDMR (RS-HDMR) has recently become a popular tool for building metamodels [9]. [10] developed a variant of RS-HDMR based on Quasi Monte Carlo (QMC) sampling. RS(QRS)-HDMR can also be used for GSA. This approach to GSA is considerably cheaper than the traditional variance-based methods in terms of computational time. However, it can only provide estimates of the first order effects and low-order interactions (up to third). There is therefore a need for the development of an efficient method for low cost estimates of the total SI's. In particular, the computational cost of estimating total SI's for all input variables should be independent of the number of model inputs. We present a method for the calculation of an upper bound on the values of total SI based on RS-HDMR or other suitable metamodels. These bounds are obtained at no extra function evaluations apart from those required to build a metamodel. Numerical tests prove that the developed approach is promising.

References:

[1] A. Saltelli and S. Tarantola and F. Campolongo and M. Ratto, "Sensitivity Analysis in Practice", *Wiley*, 2004.
[2] S. Tarantola and D. Gatelli and T. Mara, "Random Balance Designs for the Estimation of First Order Global Sensitivity Indices", *Reliability Engineering and System Safety*, **91**:717-727, 2006.
[3] J.E. Oakley and A. OHagan, "Probabilistic sensitivity analysis of complex models: a bayesian approach", *Journal of the Royal Statistical Society Series B*, **66**:751-769, 2004.
[4] B. Iooss and A. Marrel and S. Da Veiga and M. Ribatet, "Global sensitivity analysis of stochastic computer models with joint metamodels", *Stat. Comput.*, DOI 10.1007/s11222- 011-9274-8, 2011.
[5] S. Da Veiga and F. Wahl and F. Gamboa, "Local polynomial estimation for sensitivity analysis

on models with correlated inputs", *Technometrics*, **59**(4):452-463,2006.
[6] G. Li and J. Hu and S-W. Wang and P.G. Georgopoulos and J. Schoendorf and H. Rabitz, "Random Sampling-High Dimensional Model Representation (RS-HDMR) and Orthogonality of Its Different Order Component Functions", *Journal of Physical Chemistry A*, **110**(7):2474-2485, 2006.
[7] G. Li and S-W. Wang and H. Rabitz, "Practical Approaches To Construct RS-HDMR Component Functions", *Journal of Physical Chemistry A*, **106**:8721-8733, 2002.
[8] G. Blatman and B. Sudret, "Adaptive sparse polynomial chaos expansion based on least angle regression", *J. Comput. Phys.* **230**: 2345-2367, 2011.
[9] T. Ziehn and A.S. Tomlin, "Global sensitivity analysis of a 3D street canyon model-Part I: The development of high dimensional model representations", *Atmospheric Environment*, **42**(8):1857–1873, 2008.
[10] B. Feil and S. Kucherenko and N. Shah, "Comparison of Monte Carlo and Quasi Monte Carlo Sampling Methods in High Dimensional Model Representation", *Proceedings of the 2009 First International Conference on Advances in System Simulation*, 112–118, 2009.

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Assessing the convergence of a Morris-like screening method for a complex environmental model

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In environmental modelling, sensitivity analysis (SA) is very often applied to allow a dimensionality reduction of the parameter estimation problem. Due to the complexity and high computational demand of many environmental models, it is mostly impossible to use variance based methods. As a consequence, it is more common to apply screening methods for this task, like the Morris method [1] or the Latin-Hypercube – One-factor-at-A-Time (LH-OAT) technique [2]. In general, these screening methods are conceptually simple and can yield qualitative SA results (e.g. parameter rankings) with only a limited number of model evaluations. They are also particularly suited to identify model parameters for Factor Fixing (FF), i.e. putting those parameters that have no influence at all on the model output (elementary effect equal to 0) to a certain value [3].

Besides the non-influential factors, modellers also regularly fix a number of parameters that do have a (major or minor) influence on the model output to a chosen value, in order to additionally simplify the parameter estimation problem of an over-parameterized model. Hence, only the parameters that have the highest influence according to the ranking inferred with the screening method are considered in the optimization, leading to an (important) loss of model output variability.

Since it has been shown [4] that for a Morris-like screening SA with a standard number of 5 to 10 "trajectories" [5] the parameter rankings do not converge, any selection of the parameters included in the estimation process becomes questionable. In addition, a drawback of screening methods is that they can be prone to type II errors (i.e. failing to identify a factor with considerable influence on the model) [6]. Therefore, the more the parameter rankings are mixed up and facing type II errors, the higher the chance to exclude an influential parameter from the optimization and the lower the model output variance might become.

This study provides a methodology to assess the convergence of the SA results of a Morris-like screening method and shows that the number of trajectories needed to screen the parameter hyperspace of a complex environmental model should be higher than 100 to achieve converged results and parameter rankings. Moreover, it is shown that with this higher number of trajectories, the screening methods become more resilient to type II errors.

To achieve these results, the parameter sensitivities of the Soil and Water Assessment Tool (SWAT) [7] have been investigated for 2 case studies, by performing a screening with the LH-OAT technique. For both applications of this complex, computationally expensive and over-parameterized environmental model, a large set of model parameters has been included in the SA (resp. 40 and 26) and different variables have been considered as model output (discharge, suspended sediment, nitrogen concentrations, etc.). The convergence of the SA results has been tested by examining the influence of an increasing base sample size (i.e. an increasing number of trajectories), on the evolution of the mean and the variance of the elementary effects. The latter statistics are the principal sensitivity measures of Morris-like screening methods. To enhance the reliability of the convergence results, 95% confidence intervals (CIs) are assessed for the values of the mean and the variance, by performing bootstrapping with resampling [8]. The evolution of these CIs provides an additional measure to evaluate the convergence of the SA results.

References:

[1] Morris, M.D., "Factorial Sampling Plans for Preliminary Computational Experiments", *Technometrics*, **33**(2): 161–174, 1991.

[2] van Griensven, A., T. Meixner, S. Grunwald, T. Bishop, A. Diluzio and R. Srinivasan, "A global sensitivity analysis tool for the parameters of multi-variable catchment models", *Journal of Hydrology*, **324**(1–4): 10–23, 2006.

[3] Saltelli, A., S. Tarantola, F. Campolongo and M. Ratto, "Sensitivity analysis in practice - A guide to Assessing Scientific Models", *John Wiley & Sons, Ltd., Chichester*, pp232, 2009.

[4] Nossent, J. and W. Bauwens, "Multi-variable sensitivity and identifiability analysis for a complex environmental model in view of integrated water quantity and water quality modeling", *Water Science and Technology*, **65**(3): 539–549, 2012.

[5] Campolongo, F., A. Saltelli and J. Cariboni, "From screening to quantitative sensitivity analysis. A unified approach", *Computer Physics Communications*, **182**(4): 978–988, 2011.

[6] Campolongo, F. and A. Saltelli, "Sensitivity analysis of an environmental model an application of different analysis methods", *Reliability Engineering & System Safety*, **57**(1): 49–69, 1997.

[7] Arnold, J.G., P.M. Allen and G. Bernhardt, "A Comprehensive Surface-Groundwater Flow Model", *Journal of Hydrology*, **142**(1-4): 47–69, 1993.

[8] Efron, B. and R. Tibshirani, "An introduction to the bootstrap, In: CRC Monographs on Statistics & Applied Probability, eds. Cox, C.R., D.V. Hinkley, N. Reid, D.B. Rubin and B.W. Silverman" *Chapman Hall, New York*, pp456, 1993.

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Fallacies of rankings and ratings

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Abstract

According to many – including some of the authors of the Stiglitz report – composite indicators have serious shortcomings. Still these measures are pervasive in the public discourse and represent perhaps the best known face of statistics in the eyes of the general public and media. The present study delves into the potential fallacies of rankings and ratings built as arithmetic averages.

In mathematical terms, a composite indicator score (or rank) is a function of indicators and weights. Weights may represent the relative importance of each indicator or be implied by the data. The function may involve linear or geometric averaging or use of outscoring matrix in a multi-criteria setting. In their simplest and most frequent form, composite indicators are built by simply averaging normalised values across a set of indicators assuming equal weights within and across the main dimensions of the index. Yet, the weights assigned by the developers do not always coincide with the impact of an indicator to the overall index.

The paper proposes to measure the importance of a given variable within existing composite indicators via Karl Pearson's 'correlation ratio' (or 'main effect'). This measure of importance is appealing because:

- it offers a precise definition of importance, that is 'the expected reduction in variance of the composite indicator that would be obtained if a variable could be fixed';
- it can be used regardless of the degree of correlation between variables;
- it is model-free, in that it can be applied also in non-linear aggregations;
- it is not invasive, in that no changes are made to the composite indicator or to the correlation structure of the indicators (unlike the classical perturbations induced during an uncertainty analysis).

Because socio-economic variables are heteroskedastic and correlated, relative nominal weights are hardly ever found to match relative main effects; the paper proposes to summarize their discrepancy with a divergence measure. It is discussed to what extent the mapping from nominal weights to main effects can be inverted. This analysis is applied to six composite indicators, including the Human Development Index and two popular league tables of university performance. It is found that in many cases the declared importance of single indicators and their main effect are very different, and that the data correlation structure often prevents developers from obtaining the stated importance, even when modifying the nominal weights in the set of nonnegative numbers with unit sum.

The paper is addressed both to those who develop and use rankings and ratings, aiming to induce a deeper reflection on the cost of the simplification achieved with arithmetic averages.

References:

[1] Paruolo P., Saisana M., Saltelli A., "Ratin s and Rankin s: voodoo or science?", J Royal Statistical Society, **A176**(2), 2013.

[2] Saisana M., Saltelli A., "JRC audit on the 2012 WJP Rule of Law Index", In A rast, M., otero, J., Martinez, J., Ponce, A., & Pratt, C. WJP Rule of Law Index® 2012. Washington, D.C.: The World Justice Project, 2012.

[3] Saisana M., Philippas D., "Sustainable Society Index (SSI): Takin societies' pulse alon social, environmental and economic issues", EUR 2557 , Joint Research Centre, Publications Office of the European Union, Italy, 2012.

[4] Saisana M., D'Hombres ., Saltelli A., "Rickety Numbers: Volatility of university rankin s and policy implications", Research Policy, **40**:165–177, 2011.

[5] Saisana M., Saltelli A., Tarantola S., "Uncertainty and sensitivity analysis techniques as tools for the analysis and validation of composite indicators". J Royal Statistical Society, **A168**(2):307-323, 2005.

[6] OECD/JRC, "Handbook on Constructin Composite Indicators. Methodolo y and user Guide", OECD Publishing, ISBN 978-92-64-04345-9, 2008.

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Hiking to Mount Toblerone: Advanced Methods for Random Balance Design

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We present some advanced techniques which can be realized with Random Balance Design (RBD) [4] for the computation of variance based sensitivity indices enhancing the precision of the first order effect calculation.

The classical RBD method suffers from two classes of problems

- the computed values are biased with respect to the analytical values,
- the sample design in use is not necessarily exhausting the sample space (i.e., it is unclear if the design is space filling).

A freedom of choice in the design of a RBD input sample is given by the choice of the permutations. The standard RBD algorithm uses random permutations. We investigate if a clever choice of these permutation leads to a space-filling design and pays off in terms of numerical precision.

Here, the permutations used to create the realizations of the input parameters are constructed from multi-dimensional quasi-Monte-Carlo (QMC) sequences. Those are then called quasi-random permutations. For this approach, note that the map $\varphi : u \mapsto 1 - |2u - 1|$ transforms $u = (\frac{2i-1}{2n})$, $i = 1, \ldots, n$ into a sample which is useable for RBD. Now, applying the same transformation per dimension to a Latin Hypercube with conditional median (middle-of-box) placement also yields a RBD sample. If the hypercube has additional properties like low-discrepancy the RBD sample inherits this. We discuss how to exploit Sobol' LPτ sequences [3] in order to create RBD samples from quasi-random permutations. We test different quasi random sequence generators and compare their results. A discussion of convergence rates when using such a periodic quasi-Monte Carlo sample can be found in [1].

For bias reduction we investigate two strategies: the use of bias-reducing formulas which take the number of degrees of freedom into account and bootstrap methods. The bias-reducing formula has been recently discussed in [5]. A bias-reducing bootstrap estimator is available in [2]. For bootstrapping, note that $\varphi(u_i)$ and $\varphi(u_{n+1-i})$ are the same. A bootstrap method therefore may draw from these two associated outputs.

We report results on a practical example discussing the thermal energy consumption of a building.

References:

[1] L. L. Cristea, J. Dick, G. Leobacher, and F. Pillichshammer. The tent transformation can improve the convergence rate of quasi-monte carlo algorithms using digital nets. *Numer. Math.*, 105:413–455, 2007.

[2] B. Efron and G. Gong. A leisurely look at the bootstrap, the jackknife, and cross-validation. *The American Statistician*, 37(1):36–48, 1983.

[3] I. M. Sobol'. On the systematic search in a hypercube. *SIAM J. Numer. Anal.*, 16(5):790–793, 1979.

[4] S. Tarantola, D. Gatelli, and T. A. Mara. Random balance designs for the estimation of first order global sensitivity indices. *Reliab. Eng. Syst. Saf.*, 91:717–727, 2006.

[5] J.-Y. Tissot and C. Prieur. Bias correction for the estimation of sensitivity indices based on random balance designs. *Reliab. Eng. Syst. Saf.*, 107:205–213, 2012.

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Estimating Sobol' indices combining Monte Carlo estimators and Latin hypercube sampling

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Sobol' indices (SI) (Sobol', 1993) are quantities defined by normalizing parts of variance in an ANOVA decomposition (Hoeffding, 1948; Efron and Stein, 1981; Sobol', 1993). They are an important tool to study the sensitivity of a model output subject to the input parameters since they allow to quantify the relative importance of input factors of a function over their entire range of values. As they essentially consist of integrals, their computation can become rapidly expensive when the number of factors increases. Many techniques have been proposed to estimate these indices including Fast Amplitude Sensitivity Test (FAST) due to Cukier et al. (1973, 1978) and further developed by Saltelli et al. (1999), Random Balance Design (RBD) due to Tarantola et al. (2006), polynomial chaos expansion (PCE)-based estimators developed by Sudret (2008) and Blatman and Sudret (2010) and the method in Sobol' (1993). A recent review of these methods can be found in Saltelli et al. (2008), and more specifically a new introduction to FAST and RBD has been recently provided by Tissot and Prieur (2012b).

Until now, spectral methods — as FAST, RBD or PCE-based methods — which exploit the spectral decomposition of the model with respect to a particular multivariate basis, are generally preferred to the method of Sobol' because the latter is too expensive. However, spectral methods provide good estimations of SIs only under strong assumptions on the spectral decomposition of the model itself such as a decay of the spectrum sufficiently fast, the negligibility of high-order spectral coefficients, etc. As a result, these methods are not robust to complex phenomena as high-frequency variations or discontinuities, and so the method of Sobol' appears as the main method one can trust when no strong a priori knowledge on the model of interest is available.

In the following, we consider a general model connecting an output $Y \in \mathbb{R}$ to independent inputs $X_1, \dots X_d$. We assume without loss of generality that, for $i = 1, \dots d$, $X_i \sim \mathcal{U}([0,1])$. We denote $Y = f(\mathbf{X}) := f(X_1, \dots, X_d)$ where f is a deterministic real valued measurable function defined on $[0,1]^d$. We assume that Y is square integrable and non deterministic ($\mathrm{Var} Y \neq 0$).

Let $\mathbf{u}$ be a subset of size 1 or 2 of $I_d := \{1, \dots, d\}$. The closed SI (Saltelli et al., 2004) of order 1 or 2 are then defined as

$$S_{\mathbf{u}} := \frac{\mathrm{Var}(\mathbb{E}(Y|X_i, i \in u))}{\mathrm{Var}(Y)}.$$

For $\mathbf{X}$ and for any subset $\mathbf{u}$ of I_d we define $\mathbf{X}^{\mathbf{u}}$ as the d-dimensional vector such that $X_i^{\mathbf{u}} = X_i$ if $i \in \mathbf{u}$ and $X_i^{\mathbf{u}} = X_i'$ if $i \notin \mathbf{u}$ where $\mathbf{X}'$ is an independent copy of $\mathbf{X}$. We then set $Y^{\mathbf{u}} := f(\mathbf{X}^{\mathbf{u}})$.

In the following we consider two independent and identically distributed samples of the distribution of $\mathbf{X}$ — $\{\mathbf{X}_j\}_{j=1,\dots,N}$ and $\{\mathbf{X}'_j\}_{j=1,\dots,N}$ — and define for $j = 1, \dots, N$ Y_j and $Y_j^{\mathbf{u}}$ as above.

Monod et al. (2006) introduced then the following estimator whose statistical properties have been studied in Janon et al. (2012):

$$T_N^{\mathbf{u}} = \frac{\frac{1}{N}\sum_{j=1}^N Y_j Y_j^{\mathbf{u}} - \left(\frac{1}{N}\sum_{j=1}^N \left[\frac{Y_j + Y_j^{\mathbf{u}}}{2}\right]\right)^2}{\frac{1}{N}\sum_{j=1}^N \left[\frac{Y_j^2 + (Y_j^{\mathbf{u}})^2}{2}\right] - \left(\frac{1}{N}\sum_{j=1}^N \left[\frac{Y_j + Y_j^{\mathbf{u}}}{2}\right]\right)^2}.$$

Estimating all first order sensitivity indices by this approach requires $(d+1)N$ evaluations of the model, which can be quite prohibitive for costly models in high dimension.

In this talk we propose to replace the two independent samples — $\{\mathbf{X}_j\}_{j=1,\dots,N}$ and $\{\mathbf{X}'_j\}_{j=1,\dots,N}$ — by two replicated latin hypercubes of size N. We will explain how this trick allows estimating all first order SI with only $2N$ evaluations of the model. We will also present convergence results as

N tends to infinity as far as a generalization for the estimation of second order closed SI, making use of replicated orthogonal array-based latin hypercubes of strength 2 introduced in Tang (1993).

We refer to Tissot and Prieur (2012a) for more references.

References

Blatman, G. and Sudret, B. (2010). Efficient computation of global sensitivity indices using sparse polynomial chaos expansions. *Reliability Engineering and System Safety*, 95:1216–1229.

Cukier, R. I., Fortuin, C. M., Shuler, K. E., Petschek, A. G., and Schaibly, J. H. (1973). Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients: Theory. *Journal of Chemical Physics*, 59:3873–3878.

Cukier, R. I., Levine, H. B., and Shuler, K. E. (1978). Nonlinear sensitivity analysis of multiparameter model systems. *Journal of Computational Physics*, 26:1–42.

Efron, B. and Stein, C. (1981). The jackknife estimate of variance. *The Annals of Statistics*, 9(3):586–596.

Hoeffding, W. F. (1948). A class of statistics with asymptotically normal distributions. *Annals of Mathematical Statistics*, 19:293–325.

Janon, A., Klein, T., Lagnoux, A., Nodet, M., and Prieur, C. (2012+). Asymptotic normality and efficiency of two sobol index estimators. *Preprint available at http://hal.inria.fr/docs/00/66/50/48/PDF/ArtAsymptSobol.pdf.*

Monod, H., Naud, C., and Makowski, D. (2006). Uncertainty and sensitivity analysis for crop models. In Wallach, D., Makowski, D., and Jones, J. W., editors, *Working with Dynamic Crop Models: Evaluation, Analysis, Parameterization, and Applications*, chapter 4, pages 55–99. Elsevier, Amsterdam.

Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Saisana, D. G. M., and Tarantola, S. (2008). *Global Sensitivity Analysis: The Primer*. John Wiley & Sons.

Saltelli, A., Tarantola, S., and Chan, K. P. S. (1999). A quantitative model-independent method for global sensitivity analysis of model output. *Technometrics*, 41:39–56.

Saltelli, A., Tarantola, S., F., C., and M., R. (2004). Sensitivity analysis in practice: a guide to assessing scientific models.

Sobol', I. M. (1993). Sensitivity analysis for nonlinear mathematical models. *Mathematical Modeling and Computational Experiment*, 1:407–414.

Sudret, B. (2008). Global sensitivity analysis using polynomial chaos expansions. *Reliability Engineering and System Safety*, 93:964–979.

Tang, B. (1993). Orthogonal array-based latin hypercubes. *J. Amer. Statist. Assoc.*, 88:1392–1397.

Tarantola, S., Gatelli, D., and Mara, T. A. (2006). Random balance designs for the estimation of first-order global sensitivity indices. *Reliability Engineering and System Safety*, 91:717–727.

Tissot, J. Y. and Prieur, C. (2012a). Estimating Sobol' indices combining Monte Carlo estimators and Latin hypercube sampling. *Preprint available at* `http://hal.archives-ouvertes.fr/hal-00743964`.

Tissot, J. Y. and Prieur, C. (2012b). Variance-based sensitivity analysis using harmonic analysis. *Preprint avalaible at http://hal.archives-ouvertes.fr/docs/00/68/07/25/PDF/ FAST_RBD_revisited.pdf.*

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New Sensitivity Indices Subordinated to a Contrast

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For more than one decade the uncertainty propagation and the sensitivity analysis are widely used to handle mathematical models of industrial problems involving many parameters or variables: geophysics and oil reservoir, safety in nuclear industry, soil pollution, and more generally domains where it can be found heavy computation codes with large number of inputs and complex computations so that only few simulations of these codes can be run.

The uncertainty propagation uses random variables as inputs, even for deterministic codes, and study the distribution (or some characteristics) of the output. It is justified on one hand by the poor knowledge of the input parameter (or variables) and on the other hand by the relatively small number of observed output available.

Very often some of the input variables strongly affect the output (or a characteristic), while others have a small effect, and even no effect. The sensitivity analysis try to quantify these effects.

In 1993 I.M. Sobol defined indices, now called Sobol indices [1], based on the decomposition of the output variance. Using the ANOVA decomposition of a function of several variables he defined global and partial indices for single or group of variables.

In this paper we propose new global indices for one variable which generalize the Sobol ones. Indeed, it is well known that Sobol indices provide information in "central trend" in that these indices may have no meaning when considering sensitivity to extreme cases for instance. We aim at extending the Sobol indices to various kinds of trends so as to make relevant the sensitivity analysis in the context of interest.

In a numerical model $Y = h(X_1, \dots, X_p)$ the first order global sobol indices quantify the influence of a random variable X_i on the output Y, and is given by

$$S_i = \frac{\operatorname{var}(\mathbb{E}[Y|X_i])}{\operatorname{var} Y} = \frac{\operatorname{var} Y - \mathbb{E}(\operatorname{var}[Y|X_i])}{\operatorname{var} Y}.$$

The key point of our method is the following: we start from the right hand side writing of the previous index S_i, which highlights a kind of "variance differentiation". We adopt the formalism introduced in the work of N. Rachdi et al. [1] and we propose new sensitivity indices following this idea of "differentiation" but based on more general characteristics than the variance one. We denote such indices by S_i^{Ψ}, where Ψ is the *contrast* associated to the characteristic of interest, which satisfy $S_i^{\Psi} \in [0, 1]$ for all $i = 1, \dots, p$.

For example, let $Y = X_1 + X_2$, where $X_1 \sim Exp(1)$ and $X_2 \sim -X_1$, with X_1 and X_2 independent. The variable Y has the Laplace distribution with parameter 1 and its density with respect to the Lebesgue's measure is $f(x) = \exp(-|x|)/2$ (see Figure 1(left)).
The characteristic of interest is the α-quantile $q_Y(\alpha)$ of Y, hence we are seeking representative indices quantifying the influence of X_1 and X_2 on $q_Y(\alpha)$. Sobol indices give trivially $S_1^{sob} = S_1^{sob} = 0.5$ which means that X_1 and X_2 have the same influence on Y, but one certainly has the intuition that these variables do not have the same impact on extreme values of Y for instance. In Figure 1(right), we plot our new indices $S_1^{\Psi}(\alpha)$ and $S_2^{\Psi}(\alpha)$ depending on the quantile level α which gives

expected and interpretable results: the variable X_1 is the most influential when $\alpha \geq 0.5$ (the right distribution tail) and X_2 is the most influent when $\alpha \leq 0.5$ (the left distribution tail).

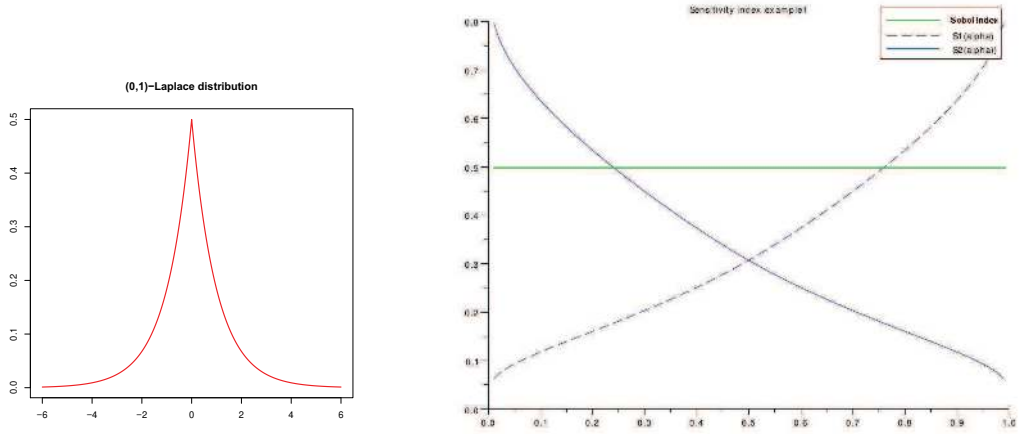

Figure 1: Left : Plot of (0,1)-Laplace distribution - Right : Sensitivity Indices, Sobol indices are in green, the blue dashed line corresponds to the index $S_1^{\Psi}(\alpha)$ that is the influence of the variable X_1 on the quantile of Y of level α, noted $q_Y(\alpha)$. The blue solid line is the influence of the variable X_2 on $q_Y(\alpha)$.

We illustrate our purpose with other academic examples and by an analytic aeronautic model which provide promising results.

References:

[1] N. Rachdi, J-C. Fort & T. Klein, "Risk bounds for new M-estimation problems", *to appear in ESAIM : Probability & Statistics*

[2] I. M. Sobol', "Sensitivity analysis for nonlinear mathematical models", *Mathematical Modeling and Computational Experiment*, **1**:407–414, 1993

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Derivative-based global sensitivity measures for interactions

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Sobol and Kucherenko [11] have recently introduced the derivative-based global sensitivity measure (DGSM), defined as the integral of the squared derivatives of the model output. These indices can be helpful when the problem dimension is large (more than ten) or when the gradient is available (or at least estimated by a finite-differences technique). Indeed, this kind of indices have been shown to be easily and efficiently estimable by sampling techniques as Monte Carlo or quasi-Monte Carlo, gaining potentially a factor ranging between 10 to 100 compared to Sobol' indices estimated with the same technique [7]. Moreover, if the computer model proposes the adjoint code to compute output derivatives [1], DGSM computations will be independent of the number of input parameters and sensitivity analysis can then be performed for models including several hundreds of inputs. Automatic differentiation tools can be helpful to that purpose [4].

A link between DGSM and Sobol' indices, given initially for the uniform and normal measure, is known for continuous probability measures: More precisely, Lamboni et al. [8] have proved the following inequality:

$$D_j^{tot} \leq C(\mu_j) \int \left(\frac{\partial f(\mathbf{x})}{\partial x_j} \right)^2 d\mu(\mathbf{x}) \tag{1}$$

where D_j^{tot} denotes the (un-normalized) total index of variable j, $d\mu(\mathbf{x}) = d\mu_1(x_1) \dots d\mu_d(x_d)$ is the integration measure (with $\mathbf{x} = (x_1, \dots, x_d)$), and $C(\mu_j)$ is a constant depending only on μ_j. Thus, the DGSM can be used for variable screening, and may be also helpful in ranking the influential variables, as studied in [6].

In this paper we extend that approach to interactions. Hence, we prove the following generalization of Inequality (1):

$$D_{i,j} \leq D_{i,j}^{superset} \leq C(\mu_i)C(\mu_j) \int \left(\frac{\partial^2 f(\mathbf{x})}{\partial x_i \partial x_j} \right)^2 d\mu(\mathbf{x}) \tag{2}$$

where $D_{i,j}$ is the second order interaction index of variables i and j, and $D_{i,j}^{superset} := \sum_{I \supseteq \{i,j\}} D_I$ is the *superset importance* [9] defined as the sum of Sobol' indices of supersets of $\{i, j\}$.

Thus, the second order derivatives contained in the Hessian of the model output are useful to investigate interactions. Such a link was investigated for instance by [2] in the context of statistical learning, but the connection to superset indices gives an original interpretation of it. While it is rare in practice that second order derivatives of the model output are directly available, they can be computed by second order finite differences. Indeed, it requires only one additive run of the model to compute a second order derivative than a first order one. Another solution would be to use automatic differentiation when possible.

The most striking application of Inequality (2) is for interaction screening: A zero value of the (squared integrated) cross derivatives indicates that there is no interaction between i and j in any order of interaction. This can be used to identify additive structures in machine learning or computer experiments [5][10][3], which can substantially improve the model performances in prediction [10]. The interaction structure can furthermore be displayed by a mathematical graph showing the active interactions as edges.

In the same vein of [8], we also investigate by numerical tests the utility of Inequality (2) in ranking the most influential interactions. While this ranking may be useful at first sight for superset importances more than for second order interactions, we can argue that in practice it is very often the case that second order interactions are the only active ones, implying that $D_{i,j} = D_{i,j}^{superset}$.

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References:

[1] D.G. Cacuci, "Sensitivity and uncertainty analysis - Theory", *Chapman & Hall/CRC*, 2003.

[2] J.H. Friedman and B.E. Popescu, "Predictive Learning via Rule Ensembles", *The Annals of Applied Statistics*, **2(3)**: 916–954, 2008.

[3] J. Fruth, O. Roustant and S. Kuhnt, "Total interaction index: A variance-based sensitivity index for interaction screening", *Submitted*, +2013.

[4] A. Griewank and G.F. Corliss, "Automatic differentiation of algorithms: Theory, implementation and application", *SIAM, Philadelphia*, 1991.

[5] G. Hooker, "Discovering additive structure in black box functions", *Proceedings of KDD, ACM DL*, 575–580, 2004.

[6] B. Iooss, A-L. Popelin, G. Blatman, C. Ciric, F. Gamboa, S. Lacaze and M. Lamboni, "Some new insights in derivative-based global sensitivity measures", *Proceedings of PSAM 11 & ESREL 2012 Conference*, 1094–1104, Helsinki, Finland, June 2012.

[7] S. Kucherenko, M. Rodriguez-Fernandez, C. Pantelides, and N. Shah. Monte Carlo evaluation of derivative-based global sensitivity measures. *Reliability Engineering and System Safety*, **94**:1135–1148, 2009.

[8] M. Lamboni, B. Iooss, A.-L. Popelin and F. Gamboa, "Derivative-based global sensitivity measures: General links with Sobol' indices and numerical tests", *Mathematics and Computers in Simulation*, **87**:45–54, 2013.

[9] R. Liu and A. Owen, "Estimating mean dimensionality of analysis of variance decompositions", *Journal of the American Statistical Association*, **101**:712–721, 2006.

[10] T. Muehlenstaedt, O. Roustant, L. Carraro and S. Kuhnt, "Data-driven kriging models based on FANOVA-decomposition", *Statistics and Computing*, **22**:723–738, 2012.

[11] I.M. Sobol and S. Kucherenko, "Derivative-based global sensitivity measures and the link with global sensitivity indices", *Mathematics and Computers in Simulation*, **79**:3009–3017, 2009.

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Estimating sensitivity indices using contribution to the sample mean

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Let $Y=f(X)$ be a function defined over a set of k input factors $X=(X_1,X_2, \ , \ _k)$ and Y is a scalar output variable obtained by evaluating the function f over X. The input factors X are uncertain and, consequently, Y is uncertain as well. We thus consider input factors $(X_1,X_2, \ , \ _k)$ as independent random variables, with pdf p_i and cdf F_i. The output Y is also a random variable. We are interested in estimating the first order indices S_i using an approach based on the contribution to the sample mean (CSM) [1].

The CSM represents the fraction of the output mean due to any given fraction of smallest values of the input X_i. Usually, CSM is plotted against the values of the cumulative distribution of X_i, which also lie in the interval [0,1]. More precisely, let consider a given quantile q in [0;1], and $F_i^{-1}(q)$ the associated value for input factor X_i. The contribution to the sample mean for input factor X_i at quantile q, denoted by $CSM_i(q)$, is defined as:

$$CSM_i(q) = \frac{1}{E(Y)} \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{F_i^{-1}(q)} \cdots \int_{-\infty}^{+\infty} f(x_1,\cdots,x_k)\left(\prod_{j=1}^{k} p_j(x_j)\right) dx_1 \cdots dx_k$$

An estimation of CSM can be constructed starting from any given sample of X and evaluating the model at any sample point. No particular sample design of X is required to estimate CSM.

In this paper, we prove that CSM has an analytical relation with the first order index S_i :

$$S_i = \frac{1}{c_v(Y)} \cdot \int_0^1 \left(\frac{dCSM_i}{dq}(q) - 1 \right)^2 dq$$

This fact enables us to estimate S_i using CSM points. Therefore, the estimation of S_i can be made from any given sample. We test the proposed approach against other existing approaches for estimation of S_i with given samples.

References :

[1] Bolado-Lavin, R., W. Castaings and S. Tarantola, "Contribution to the sample mean plot for graphical and numerical sensitivity analysis", Reliab. Eng. Syst. Safe., **94**, 1041-1049, 2009

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Sensitivity Analysis of Final Repository Models Using Quasi-Random Sampling and a Metamodel Approach.

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Performance Assessment (PA) models for radioactive waste repositories include a variety of coupled flow, transport and chemical processes. Such models often show a highly non-linear and non-monotonic behaviour, highly skewed and heavily tailed model outputs and significant parameter interactions. The computational effort for a robust and reliable sensitivity analysis may be significantly reduced by using quasi-Monte-Carlo (QMC) sampling and metamodels. Quasi-Monte-Carlo sampling methods are also often called quasi-random sampling or low discrepancy sequences. Discrepancy is a measure of how uniformly a set of points fills an area of multidimensional space. Consequently, in a low discrepancy sequence, the points are as equally spaced as possible [1]. A metamodel is a surrogate model that emulates the behaviour of the original model as closely as possible with a low computational effort. Once assembled, the metamodel can be used to estimate the sensitivity indices of the original model with lower CPU costs. This study investigates the performance and efficiency of LpTau low discrepancy sampling [2] compared with random and Latin Hypercube type sampling techniques. In connection with the different sampling techniques, the performance of the State-Dependent-Parameter (SDP) metamodel [3] is evaluated and compared to that of EFAST. The resulting parameter rankings are compared to those provided by the Standardised Rank Regression Coefficients (SRRC) and the Contribution to the Sample Mean (CSM) plots. Effects of the sample sizes are also examined. Initial results indicate best convergence of the SDP method as well as the CSM plots and the SRRC method if combined with the LpTau sampling method. The EFAST method, however, seems to have some convergence problems.

Keywords :

Low discrepancy sequence; LpTau sampling method; State-Dependent-Parameter (SDP) method; Performance Assessment (PA) models for radioactive waste repositories; Contribution to the Sample Mean (CSM) plots

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References :

[1] NAG Numerical functions for GPUs, Chapter introduction. gpu_g05 – random number generators, NP3680/0, 2005.

[2] B. Shukhman, Generation of quasi-random (LP_τ) vectors for parallel computation. Computer Physics Communications, **78**: 279-286, 1994.

[3] M. Ratto, A. Pagano and P. Young, “State dependent parameter metamodelling and sensitivity analysis”, Computer Physics Communications, **177**: 863–876, 2007.

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Derivative-based sensitivity indices based on polynomial chaos expansions

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Global sensitivity analysis has emerged in the last 15 years as a powerful tool for improving the understanding of complex environmental, industrial or civil systems. In many fields of applied and engineering sciences indeed, computer simulation models are now inescapable. The increasing computer power which is available through large clusters of CPUs has made it possible to develop models with increasing fidelity (*e.g.* accounting for physical couplings) at the price of an increasing number of input parameters. In practice most of the parameters (corresponding for instance to initial or boundary conditions for evolutionary systems) are not well known. A probabilistic approach is then suitable for modelling the uncertainties about these parameters. Then the question of the relative impact of these uncertainties onto the model predictions naturally arises.

Global sensitivity analysis aims at determining which input parameters of the model (resp. which combination of input parameters) have the greatest influence on the variability of the model output [1]. Several methods are now well established depending on the type of information that is required:

- Screening methods [2,3] aim at finding which parameters have no infuence on the model output at a low computational cost.
- Variance-based sensitivity indices such as the Sobol' indices aim at describing how the variance of the model output can be decomposed in terms of contributions of each input parameters or combinations thereof [4].
- Distribution-based sensitivity indices quantify how much the distribution of the output changes when some input parameters are fixed [5,6].
- Derivative based sensitivity indices that have been recently proposed in [7,8] may be viewed as a generalization of Morris importance measure.

In the context of industrial applications the computation budget, *i.e.* the number of affordable runs of the computational model that is allowed to evaluate the sensitivity indices is rather low, typically less than 1,000. Thus the classical Monte Carlo-based estimators of the various sensitivity indices listed above are not applicable.

In this paper we will concentrate on the last category of indices, namely the derivative-based sensitivity indices. Consider a random vector $\boldsymbol{X}$ of dimension M with independent components and joint probability density function $f_{\boldsymbol{X}}$. Let us denote by $Y = \mathcal{M}(\boldsymbol{X})$ the random response of the simulation model of interest. The derivative based sensitivity indices (DGSM) are defined by:

$$\nu_j = \mathbb{E}\left[\left(\frac{\partial \mathcal{M}}{\partial x_j}(\boldsymbol{X})\right)^2\right] \tag{1}$$

In order to efficiently compute them efficiently a *polynomial chaos expansion* of the model output is used [9]:

$$Y = \sum_{\boldsymbol{\alpha}\in\mathbb{N}^M} a_{\boldsymbol{\alpha}}\, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \tag{2}$$

where $\Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$ are multivariate orthonormal polynomials with respect to the probability measure associated with random vector $\boldsymbol{X}$. In the present paper we use *sparse* polynomial chaos expansions whose basis functions are selected using the Least Angle regression algorithm [10,11].

The accuracy of the sparse polynomial chaos expansion is checked by a leave-one-out cross-validation procedure. Once a sufficient accuracy has been obtained, the PC expansion is post-processed in order to compute the derivative-based sensitivity indices. The very polynomial nature of the expansion makes it possible to compute *analytically* the derivatives of the PC expansions.

The proposed approach is illustrated on several application examples that have been addressed in the recent literature, especially in [8,12]. The convergence of the indices as a function of the global leave-one-out mean square error is checked.

References:

[1] A. Saltelli, K. Chan, and E.M. Scott, editors. Sensitivity analysis. J. Wiley & Sons, 2000.

[2] M.D. Morris. Factorial sampling plans for preliminary computational experiments. Technometrics, **33**(2):161–174, 1991.

[3] F. Campolongo, A. Saltelli, and J. Cariboni. From screening to quantitative sensitivity analysis. A unified approach. Comput. Phys. Comm., **182**(4):978–988, 2011.

[4] I.M. Sobol. Sensitivity estimates for nonlinear mathematical models. Math. Modeling & Comp. Exp., **1**:407–414, 1993.

[5] E. Borgonovo. A new uncertainty importance measure. Reliab. Eng. Sys. Safety, **92**:771–784, 2007.

[6] E. Borgonovo, W. Castaings, and S. Tarantola. Moment-independent importance measures: new results and analytical test cases. Risk Analysis, **31**(3):404–428, 2011.

[7] I.M. Sobol and S. Kucherenko. Derivative based global sensitivity measures and their link with global sensitivity indices. Math. Comput. Simul., **79**(10):3009–3017, 2009.

[8] Sobol', I. and S. Kucherenko. A new derivative based importance criterion for groups of variables and its link with the global sensitivity index Comput. Phys. Comm., 2010, 181, 1212-1217

[9] B. Sudret. Global sensitivity analysis using polynomial chaos expansions. Reliab. Eng. Sys. Safety, **93**:964–979, 2008.

[10] B. Efron, T. Hastie, I. Johnstone, and R. Tibshirani. Least angle regression. Annals of Statistics, **32**:407–499, 2004.

[11] G. Blatman and B. Sudret. Adaptive sparse polynomial chaos expansion based on Least Angle Regression. J. Comput. Phys, **230**:2345–2367, 2011.

[12] M. Lamboni, B. Iooss, A.-L. Popelin, and F. Gamboa. Derivative-based global sensitivity measures: general links with Sobol' indices and numerical tests, Mathematics and Computers in Simulation, **87**:45–54, 2013.

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A sensitivity analysis of the birth cohort model for tertiary education attainment 2011-2020

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Sensitivity analysis has been established as a suitable means to understand whether models are sensitive to the underlying assumptions (cf. Leamer, 2010, and Saltelli and Annoni, 2010). A sensitivity analysis helps to uncover how uncertain a particular inference from a model is and to what extent certain input factors contribute to the uncertainty in model output. While the merits of performing a sensitivity analysis are evident, applications in the field of education models are sparse.

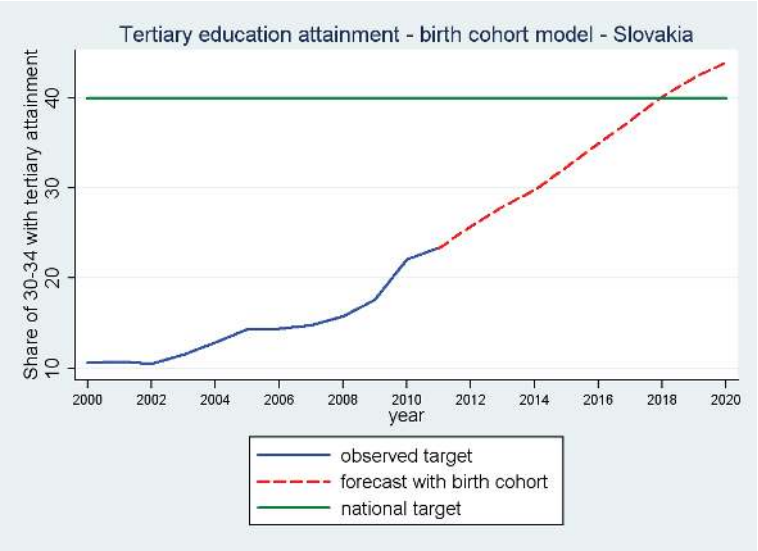
A quick literature search shows that sensitivity analysis has not been used (to the authors' knowledge) in the area of education and training. If at all, the robustness of education models is assessed by performing a 'once-at-a-time' sensitivity analysis instead of performing a simultaneous sensitivity analysis. One reason of the lack of applications of sensitivity analysis in the field of education models might be the distinct nature of those models, i.e. problems of missing or low-quality data, high complexity of the modelling structure, such as interactions between various input factors, as well as nontrivial distribution of input parameters.

This paper proposes to perform a simultaneous sensitivity analysis on an education model and thereby demonstrates how sensitivity analysis can be used to test the reliability of models in the area of education. In particular, we will perform a sensitivity analysis on the outcomes of a birth cohort model, which is used to forecast the tertiary education attainment in EU Member States from 2011 until 2020, and thereby monitors the performance of countries for the European Commission. EU member states are expected to set a national target for tertiary attainment and outline policies to achieve the target. In particular, the indicator set by the European Commission on tertiary attainment aims at increasing "the proportion of 30-34 year olds having completed tertiary or equivalent education to at least 40%" (cf. Eurostat, 2012). To understand whether countries will be able to achieve their national targets until 2020 we developed a birth cohort method, which allows forecasting the benchmark value until 2020 (see also related work on headline indicators (Badescu, D'Hombres, and Weber, 2012)). In particular, we use administrative data drawn from the UIS/OECD/EUROSTAT data collection (UOE) and construct an indicator to measure the completion by this target population by using new entrants to tertiary education by age group, the average duration of studies and the average completion rate as reported by countries. With these variables we can track individuals in different birth cohorts and based on the flow of new entrants in tertiary education, we predict the output, i.e. the proportion, in the coming years, of people aged between 30 and 34 with completed tertiary education.

In Figure 1, we applied the birth cohort method to an EU Member State, i.e. Slovakia, and show that under the base-line scenario the forecasted values (in red) are above the national target set for Slovakia (in green). However, the margin by which Slovakia is surpassing its national target is relatively small and whether a member state over- or underperforms is politically relevant and has important consequences for its country-specific recommendations issued by the European Commission.

Hence, the question remains to what extent reaching the national target depends on the underlying assumptions intrinsic to the birth cohort model. In particular, we investigate the uncertainty due to the missing data which is required to provide forecasts, using a novel approach which attempts to capture uncertainty due to extrapolation. Simultaneously, we explore the effect of the uncertainty in model parameters such as the average completion rate and duration of tertiary education. To assess sensitivity, we estimate variance-based sensitivity indices of the various sources of uncertainty using Monte Carlo integration. As a result, we are able to estimate the uncertainty in the forecasts, and to identify which model inputs are the most and least influential in determining the output uncertainty.

Figure 1: Base-line: Birth cohort calculation for Slovakia



References:

Badescu, M., D'Hombres, B., & Weber, A. (2012). *Monitoring the EU Headline Target in Education and Training - Methodology and Country Sheets.* Luxembourg: JRC Scientific and Technical Reports No. 70190.

Eurostat. (2012). *Headline Indicators*. Retrieved December 3, 2012, from http://epp.eurostat.ec.europa.eu/portal/page/portal/europe_2020_indicators/headline_indicators

Leamer, E. E. (2010). Tantalus on the Road to Asymptopia. *Journal of Economic Perspectives, 24*(2), 31-46.

Saltelli, A., & Annoni, P. (2010). How to Avoid a Perfunctory Sensitivity Analysis. *Environmental Modelling & Software, 25*(12), 1508-1517.

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Global Sensitivity Analysis for Interpretation of Black Box Functions

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Consider a smooth and continuous black box function $f(\mathbf{x})$ obtained through a machine learning technique. Such a function links an output to d input variables $\mathbf{x} \in \mathbf{R}^d$. An example of such function would be a feed-forward neural network [1],

$$f(\mathbf{x}) = b_o + \sum_{i=1}^{d} w_{i\to o} x_i + \sum_{h=1}^{H} w_{h\to o}\, \phi(b_h + \sum_{i=1}^{d} w_{i\to h} x_i)\,, \tag{1}$$

where $\phi(z) = (1+\exp(-z))^{-1}$ is the logistic function. The network is parameterized with the set of weights $\{w_{i\to o}, w_{h\to o}, w_{i\to h}\}$, and biases $\{b_o, b_h\}$. These parameters are obtained from data using the optimization algorithms especially devised for the neural network learning [1]. Although black box functions, like the neural network structure (1), are able to map input/output relations in data, they are not suitable for interpretation and sensitivity analysis. For example, it is not possible to quantify relative importance of the various inputs to the function response as well as to understand manner in which inputs affect the response: additive or also through some interactions. For the purpose of interpretation of functions like the neural network (1), it is useful to represent them using the following finite dimension-wise expansion with 2^d terms [2], i.e. the ANOVA decomposition:

$$f(\mathbf{x}) = f_0 + \sum_{\mathbf{u}\subseteq\{1,2,\ldots,d\}} f_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}})\,, \tag{2}$$

where a component function $f_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}})$ depends only on those components of input vector $\mathbf{x}$ which indices are non-zero elements in the set $\mathbf{u}$. In the notation used in (2), the summation is over all subsets $\mathbf{u}$ of the set $\{1,2,\ldots,d\}$, where the number of non-zero elements in the set $\mathbf{u}$ is less than or equal to d. Thus $\mathbf{u}$ can have 1, 2, … and up to d non-zero elements. The black box function representation (2) is unique if the line integrals of every component $f_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}})$ over any of its own variables $\mathbf{x}_{\mathbf{u}}$ are qual to zero [2]. In such an expansion all components $f_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}})$ are orthogonal. In Eq. (2) f_0 represents a constant (i.e. mean value) and one-dimensional component functions $f_{u_1}(x_{u_1})$ are referred to as the main effect of the corresponding input variable. Multi-dimensional component functions $f_{u_1,u_2}(x_{u_1},x_{u_2})$, $f_{u_1,u_2,u_3}(x_{u_1},x_{u_2},x_{u_3}),\ldots$ represent interactions between different input variables.

It often happens in practice that response of a black box function depends only on either additive inputs or low dimension interactions between input variables. Hence, the finite dimension-wise expansion (2) decays fast. Consequently the effective dimension d_{es}, in the superposition sense [3], of the function $f(\mathbf{x})$ is smaller than d, and conversion of $f(\mathbf{x})$ to the dimension-wise expansion (2) can be achieved with a truncation of the components $f_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}})$ in (2) that have cardinality of the subset $\mathbf{u}$ greater than d_{es}. In this way a high-dimensional black box $f(\mathbf{x})$ can be converted into a sequence of functions with lower dimensions. It is of great practical importance to devise a method that will exploit low effective dimension ($d_{es} < d$) when

computing variance-based sensitivity indices to be used for interpretation of black box functions (1).

The paper presents two methods which are suitable for the global sensitivity analysis of the black box functions (1). The first method, called Sparse Grid Regression [4], is based on the parameterization of the ANOVA model (2) via a linear combination of the multidimensional basis functions. These basis functions are designed through a tensor product of orthogonal polynomials. To estimate parameters we solve multi-dimensional integrals using Sparse Grid technique [5]. The global sensitivity indices [2] are used to determining effective dimension and to do shrinkage of the model (2). The same indices are used for interpretation of the black box function (1).

The second method is fundamentally different. It is based on the approximation of the black-box function (1) via Tensor Product Series [6]. The main tool in this approach is the Splitting Operator [6], which is able to replace the calculation of one integral in two dimensions by $2n$ integrals each in one dimension, where n is the rank of the Tensor Product Series. This technique is extended to multiple dimensions via recursive application of the Splitting Operator, where in each step, dimension of integrands are cut in half till the problem is reduced to some number of single dimensional integrations [7]. The paper demonstrates the application of the Splitting Operator in computing multidimensional integrals required in global sensitivity analysis of the black box function (1).

Numerical example is devised to compare efficiency and accuracy of computing sensitivity indices using Sparse Grid Regression and by using Tensor Product Series approximation. These results are also compared to the results obtained via the Quasi-Monte Carlo method.

References:

[1] W. Venables and B. Ripley, *Modern Applied Statistics with S-PLUS*, Springer, New York, 1999.
[2] I.M. Sobol, “Sensitivity estimates for non-linear mathematical models”, *Mathematical Modelling and Computational Experiment*, **1**: 407-414, 1993.
[3] R.E. Caflisch, W. Morokoff and A.B. Owen, “Valuation of mortgage backed securities using Brownian Bridges to reduce effective dimension”, *Journal of Computational Finance*, **1** (1): 27-46, 1997.
[4] R. Živanović, “Global sensitivity analysis of transmission line fault-locating algorithms using sparse grid regression”, *Reliability Engineering & System Safety*, **107**:132-138, 2012.
[5] T.Gerstner and M.Griebel, (1998): ”Numerical integration using Sparse Grids”, *Numerical Algorithms*, **18**(3-4): 209-232, 1998.
[6] F.W. Chapman, “An elementary algorithm for the automatic derivation and proof of tensor product identities via computer algebra”, *ISSAC’03*, August 3–6, 2003, Philadelphia, Pennsylvania, USA.
[7] O.A. Carvajal, F.W. Chapmana and K.O. Geddes, “Hybrid symbolic-numeric integration in multiple dimensions via Tensor-Product Series”, *ISSAC’05,* July 24–27, 2005, Beijing, China.

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