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Uncertainty and Sensitivity Analysis for policy decision making

An introductory guide

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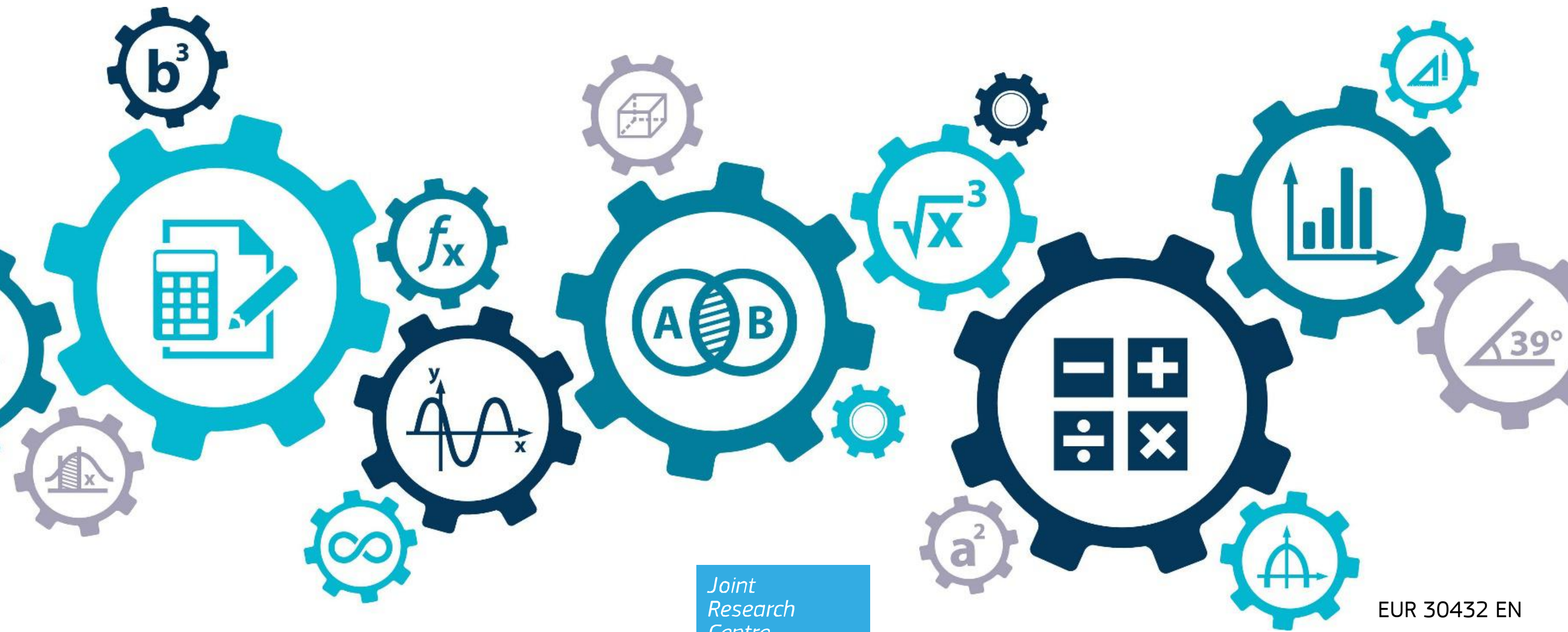
2020



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Contents

Foreword

This report is authored by the Commission Competence Centre on Modelling (CC-MOD).

CC-MOD promotes a transparent, coherent and responsible use of modelling to underpin the evidence base for EU policies.

Within CC-MOD, the Sensitivity Analysis of Model Output (SAMO) team has the mission to carry out uncertainty and sensitivity analyses of EC workhorse models, to conduct research in this field, to provide tools, training courses and ad hoc scientific support to model users in order to enhance the robustness of model-based evidence in the European Commission.

For more information on the Competence Centre on Modelling please visit https://ec.europa.eu/knowledge4policy/modelling_en

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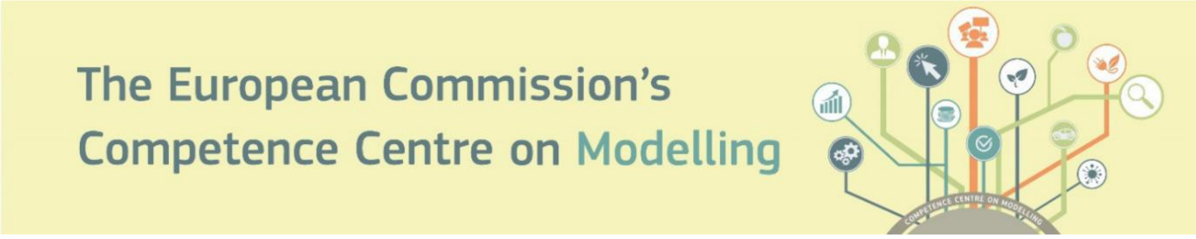
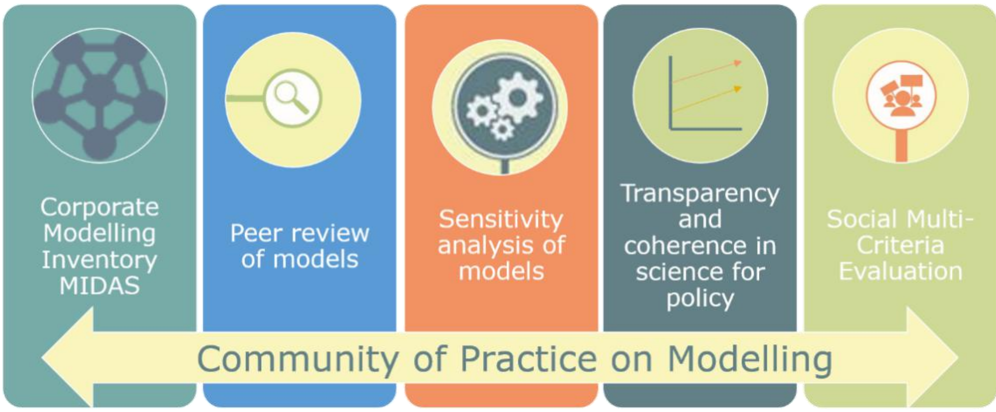


The **Competence Centre on Modelling** (CC-MOD) promotes a **responsible, coherent and transparent use of modelling** to underpin the evidence base for EU policies.

The **Commission makes extensive use of models** to support the whole policy cycle, for example in the ex-ante assessment of the environmental, economic, and social impacts of policies; to accompany policy implementation; or for ex-post policy evaluation. The **transparency, quality and coherence** of evidence in support to EU policy decisions are vital for the Commission policy analysis.

Launched in 2017, CC-MOD pools the Commission competencies and best practices in developing and using models, to help identify common approaches to quality and transparency of model use. CC-MOD facilitates dialogue between policy makers and modelling teams across the Commission and promotes the use of multi-disciplinary and integrated modelling approaches.



CC-MOD **main activities** include:

- **Management of MIDAS, the Commission corporate modelling inventory and knowledge management system**. Maintaining an overview of ongoing modelling activities is the first step for a transparent and coherent use of models in support to the policy cycle. MIDAS contains the descriptions of models in use by the Commission in support of the policy cycle. MIDAS is open to the public as of the end of 2020, giving access to the descriptions of the models contributing to Commission impact assessments.
- **Services and tools for uncertainty and sensitivity analysis.** CC-MOD provides specific support and training in the setting up and execution of uncertainty and sensitivity analyses, as well as ad-hoc support to Commission Policy Directorate – Generals (DGs) on model quality assurance. The JRC also contributes to the methodological development and the diffusion of the discipline worldwide.

- **Organization of model peer-reviews.** As part of its quality assurance and transparency tasks, CC-MOD is implementing since 2016 a peer review process for models of the Commission. The model reviews, which are undertaken by an external Review Panel, aim at improving the quality and transparency of models used for EU policy making. The Model Review Report informs about the transparency, quality and fitness for purpose of the model, and provides suggestions and recommendations for future development and use.
- **Promotion of transparency and coherence in model use.** CC-MOD seeks to advance the further development of a consistent approach towards transparency with a view to elucidate the structure and the causal mechanisms which make up a model, and the related data and information flows. CC-MOD also supports the improvement of the quality and consistency of baseline scenarios used for policy modelling at the Commission.
- **Training and ad-hoc support on social multi-criteria evaluation (SMCE) of policy options.** Multi-criteria decision analysis is the most widespread multidimensional approach to ex-ante impact assessment. SMCE, explicitly designed for public policy, is a very useful methodological and operational framework for ex-ante impact assessment. SMCE can provide a methodology which is inter/multi-disciplinary, participatory and transparent. CC-MOD activities include the development of a software tool and training courses on the use of SMCE for ex-ante impact assessment.

CC-MOD also facilitates **the Community of Practice (CoP) on Modelling**, the Commission wide network of researchers and policy makers involved in model development and use. The CoP on modeling acts as the forum for the exchange of modelling-related knowledge and best practices. The steering group of the activities of the Competence Centre and the Community of Practice is the Commission **Inter-Service Group on Modelling**.

CC-MOD contributes to the Commission's Better Regulation policy, the Inter-Institutional Agreement on Better Law Making and the Communication on Data, Information and Knowledge Management at the European Commission.

Further information on CC-MOD is available at:

https://ec.europa.eu/knowledge4policy/modelling_en
https://webgate.ec.europa.eu/connected/groups/cc-mod (Commission internal).

Abstract

The European Commission is committed to transparent and evidence based policy making throughout the policy cycle. Simulation models are increasingly used in impact assessments to provide support to policy makers across a wide range of policy areas. To ensure model quality in support to policy, understanding and communicating uncertainty in model outputs is essential. In modelling, accounting for uncertainties and identifying its most important sources is an inherent issue. Uncertainty and sensitivity analysis should be systematically performed in modelling activities in support to policy making. This report aims at highlighting the added value that uncertainty and sensitivity analysis can bring to modelling activities to inform policy makers, and presents a specific software that has been developed within the Commission to help modellers and analysts.

1 Introduction

The European Commission (EC) is committed to open and transparent decision making, to be informed by the best available understanding of policy impacts throughout the policy cycle. This approach is reflected in the Commission **Better Regulation** policy, the main regulatory framework of the EU[1].

The Better Regulation Guidelines, which provide concrete guidance on how to better apply regulation principles, recommend **quantifying policy impacts** as much as possible (European Commission 2017). In this respect, **simulation models have become increasingly important.** Models are extensively used to support the whole policy cycle, from the ex-ante assessment of the environmental, economic, and social impacts of policies, to policy implementation and ex-post evaluation.

As for all assessment methods, **understanding and communicating uncertainty** in model outputs **is vital**. Good and transparent practice in providing evidence for policy support requires that uncertainty be quantified and taken into account as much as possible. This is particularly relevant in an impact assessment (IA), as this could change the ranking and conclusions about the policy options. In this respect, **uncertainty analysis (UA) and sensitivity analysis (SA)** play a central role among the available methodologies.

This report, authored by the **Commission Competence Centre on Modelling** (CC-MOD)[2], presents a general overview and applications of how uncertainty and sensitivity analysis of model outputs can **concretely contribute to better inform the decision-making process**. CC-MOD promotes a responsible, coherent and transparent use of modelling to underpin the evidence base for EU policies.

The report is organized as follows. Section 2 introduces how UA and SA can contribute to model use for policy support, with specific reference to EC impact assessments. UA and SA are then specifically addressed in sections 3 and 4, underlying relevant aspects for model use in support to policy making. Section 5 presents an online tool, developed by CC-MOD, which can assist Commission staff for carrying out UA and SA specifically in impact assessment activities. Section 6 concludes.

The user guide for the online tool (EC WebApp) for sensitivity analysis is included in Annex 1. Its methodological foundations are explained in Annex 2, while Annex 3 provides an overview of the main sensitivity analysis methodologies.

1 Information on the Better Regulation is available at: https://ec.europa.eu/info/law/law-making-process/planning-and-proposing-law/better-regulation-why-and-how_en.

2 Information on CC-MOD is available at: https://ec.europa.eu/knowledge4policy/modelling_en.

2 Policy making and model uncertainty

Scientifically **sound evidence is essential for better policy making**. Evidence aims at informing decision makers about possible policy impacts on several aspects such as the economy, the environment, society, and health… For this purpose, when carrying out their analyses analysts have to consider the current state of knowledge and all available data. In addition, good and transparent practice in providing evidence for policy support requires that **uncertainty** is **quantified and taken into account to the extent possible**.

The complexity of political priorities of the EU Commission increasingly demands cross-cutting responses and cooperation across Directorate Generals (DGs). Therefore, EU policy making and impact assessment activities call for a diversity of knowledge and competences of DGs, external experts, and stakeholders as well as, increasingly, quantitative evidence provided by mathematical models.

A **model** can be defined as an analytical representation or quantification of a real-world system, used to make projections or to assess the behaviour of the system under specified conditions. It represents the current state of knowledge about the concerned economic, environmental, social or health system. A model is a simplification of reality usually developed to address a specific issue. Great care must be taken when models are used for policy by making sure that they are fit for the purpose. **Maximum quality, transparency and coherence are required in the use of models for policy support**. Notably, model results should be reproducible and available for scrutiny.

Simulation **models** are essential instruments in policy-making processes[3] and **are widely used in Commission impact assessment**. Indeed, 16% of all EC impact assessments carried out in the years 2003-2018 are supported by models, increasing up to 25-30% from 2015 onwards. Around 120 models have been used to this extent (Acs et al., 2019). Policy areas characterized by frequent use of models in support of EU policy making include, among others, environment, economics, energy, health, and agriculture.

Model outcomes are affected by a certain degree of uncertainty which in many cases can be very significant. Consequently, the meaning of model outputs, their possible interpretations and sources of uncertainty, and, thus, the quality of the information supporting decision processes demand some additional precautionary steps. Effective and transparent practice in providing evidence for policy support requires taking into account the impact of uncertainty on model output, and its supposed implications on policy options. Hence, the different sources of uncertainty should be identified and quantified to the extent possible, as indeed the quantification of uncertainty of model results can affect decision-makers' choices.

Acknowledging and quantifying uncertainty is a complex and multi-faceted issue, and is related to the general concept of Modelling Quality Assurance (MQA). MQA *de facto* contributes to proper and transparent use of models, and subsequently leads to improved evaluation of the impact of policy options, and thus to better evidence based policy making.

In this context, methodological approaches must support responsible use of mathematical models. Uncertainty analysis (UA) and sensitivity analysis (SA) play an important role

3 The Commission-wide Corporate modelling inventory and knowledge management system MIDAS (see Ostlaender et al., 2019) includes the descriptions of models in use by the EC in support of the policy cycle. Models can be developed by the EC or by third parties, such as national or international research institutes, companies or consortia. The JRC is a major provider of models to the EU Commission. Modelling capacities are also available in some of the policy DGs.

among the available methodologies (see Figure 1). Nowadays, they are mature disciplines, well-established and employed worldwide in different fields of investigation.

While **uncertainty analysis** aims at quantifying the uncertainty in model output due to the uncertainty in model inputs, **sensitivity analysis** establishes how the quantified uncertainty in model results can be attributed to the different sources of uncertainty in the model inputs. Uncertainty and sensitivity analyses (UA-SA) are an integral part of the modelling process (Saltelli et al., 2004).

In the remainder of this report, the application of UA and SA of model output to better inform the decision making process will be discussed.

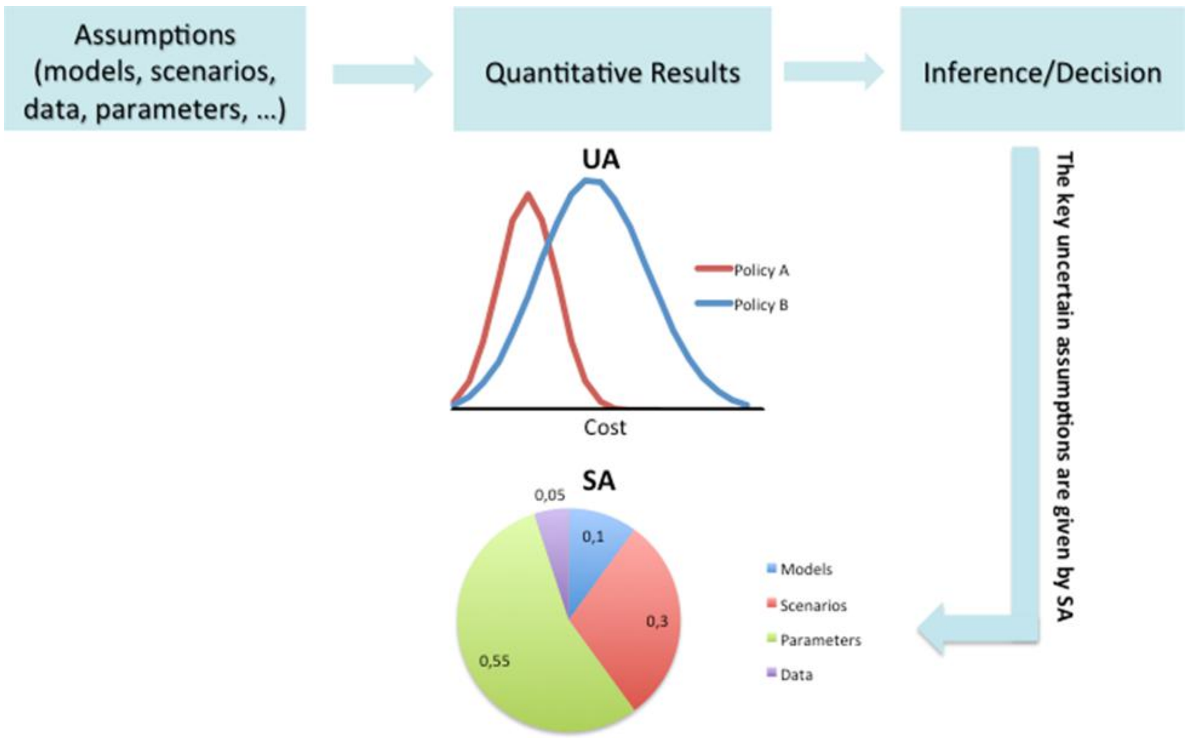


Figure 1. Informed decisions are based on scientifically sound evidence. The latter is inferred from scientific knowledge and assumptions. The assumptions (or inputs) are subject to uncertainties which should be accounted for when informing decision-makers. This is where uncertainty and sensitivity analyses come into play.

2.1 The role of uncertainty and sensitivity analysis

Models and data are subject to uncertainty, which can sometimes be irreducible and quite substantial. As the quantified impacts of policy options rely heavily on model output, the crucial question is to know how model outputs (in case of policy making, these refer to the impacts of the policy options) can be affected by these uncertainties.

In this respect, **the use of uncertainty analysis and sensitivity analysis** is **strongly recommended** by the EU Commission.

References to these methodologies can be found already in the Impact Assessment Guidelines (2009), and then in the **Better Regulation Guidelines and Toolbox** (EC, 2017), where we read that "*Whenever an assumption is particularly important or uncertain, sensitivity analysis should be used to check whether changing it would lead to significantly different results*" (Better regulation Guidelines, EC, 2017: p. 26) and "*a transparent and high-quality impact assessment should acknowledge and, to the extent relevant or possible, attempt to quantify the uncertainty in model results because the uncertainty could change the ranking and conclusions about the policy options*" (Better Regulation Toolbox EC, 2017: p. 510). Therefore, the Guidelines **recommend the use of uncertainty and sensitivity analysis** as tools for **modelling quality assurance** to check whether alternative factors (assumptions, variables, data) would lead to significantly different results, and hence to different policy impacts and possibly ranking of the policy options.

In addition to the European Commission, other national and international agencies have recognised the key role of UA-SA in model based decision making. Among them, we can cite the Intergovernmental Panel on Climate Change (Mastrandrea et al., 2010), the US Environmental Protection Agency's modelling guidelines (EPA, 2009) and the World Health Organization (WHO, 2008).

UA-SA have a consolidated tradition and their unique role in model development is widely acknowledged by modellers. UA and SA can be employed to further investigate the model itself and to better understand the relationship between model inputs and outputs. Uncertainty and sensitivity analysis can be undertaken for example for the following issues (for a broader review, see Saltelli et al., 2004):

- ranking of the inputs by order of importance to prioritize future research;
- identifying irrelevant inputs which can be fixed to their nominal values (for instance, for model calibration purposes);
- mapping of the input space that provides model responses within some desired (plausible) ranges;
- conducting *what-if analysis* which investigates what the impact on the model response of interest would be if one or several input variables were changed (w.r.t. some base case scenario);
- finding possible unexpected relationships between input and output that might pinpoint inconsistencies in the model.

UA-SA are crucial as they **help identifying the factors (assumptions, variables, data, and uncertainties) at play and provide information on their influence** in quantitatively driving the impacts of the various policy options.

In **policy decision making**, UA-SA do not limit their contribution to the development and intrinsic consideration about the models used, but extend their capacity as powerful instruments of **transparency and quality**. UA-SA are not only applicable to complex models, but also to any quantitative projections/analysis relying on uncertain assumptions and data.

UA-SA can **quantitatively explore how the policy options and impacts under analysis would change** in response to an (even slightly) different modelling assumption, or in response to variations in key variables. The relevance of the assumptions and the importance of the variables cannot always be precisely detected without such analysis. Performing sensitivity analysis methods allow to highlight which uncertain inputs are responsible for uncertainty in policy impact and can identify 'switching points' by asking which key elements (assumptions, variables, data) have to be changed (and how much) in order for the option/impact to vary. This additional knowledge is uniquely provided by UA-SA. The identification of the main drivers of the policy options/impacts confers enhanced credibility to the model and its output(s).

The result of **uncertainty analysis** can be **the identification of a policy option definitely having a positive impact** compared with the other available options. Therefore, a robust decision is possible because, in spite of the output variability, the impact of the specific policy option is to be preferred. **At the other extreme, the uncertainties might be so large that no decision can be definitely supported**.

The **sensitivity analysis provides useful information** about uncertain input relevance and key assumptions that should be better known in order to reduce the model uncertainty.

UA-SA are essential for impact assessment and **should be routinely performed by modellers/analysts**. Within the MQA paradigm, the model development phases should be integrated with some uncertainty and sensitivity analyses in an iterative process to improve model quality. In the same way, when models are used in the policy decision process, i.e. in impact assessment, UA-SA can be conducted referring to the specific assumptions and data of the policy case. It must be stressed that **the sensitivity analysis is intended to be problem-oriented and not model-oriented**. This implies that different conclusions can be reached when performing the UA-SA for impact assessments, even using the same model, if the goal and assumptions of the policy study are modified.

UA-SA should be included early in the planning of an impact assessment, in particular to be sure that the information needed for the SA exercise can be made available at the right point in time and with an efficient use of resources. Additional resources required by UA-SA should be considered as a profitable investment compared with the risk of lacking information and/or reduced quality of the analysis.

CC-MOD provides support to EU analysts/modellers to increase quality and reliability in model use. Within CC-MOD, the **Sensitivity Analysis of Model Output (SAMO) team provides guidance** and assistance in carrying out uncertainty and sensitivity analysis of model outputs for the EU Commission, and aims to promote the MQA concept through the systematic implementation of these methodologies.

2.2 Sensitivity analysis in impact assessment

EC impact assessments carried out during the period 2011-2018[4], show a **positive trend in considering sensitivity analysis**: in 2018, the percentage of impact assessments contemplating SA increased up to about 30%, whereas over the whole period the average is around 18%. Nevertheless, from the analysis it also emerges that the potential of this kind of inspection has not yet been completely and fully exploited.

Obviously, a sensitivity analysis is not always pertinent or required in impact assessment. However, the extent to which SA is performed can be improved. In addition, when SA is conducted, some further inspections are needed about the different approaches applied.

The sensitivity analyses carried out in EC impact assessments over the period considered can be classified mainly into four groups, as follows:

- **One-At-a-Time (OAT)** approach, where inputs/assumptions are changed one at a time (i.e. the minimum and the maximum values are considered) and the model outputs are compared with a given baseline (this can overlap with scenario comparison in some cases);
- **Qualitative description**, mainly based on a qualitative discussion about the most important and uncertain assumptions, without a quantitative investigation;
- **Scenario comparison**, where two or more alternative scenarios are compared (i.e. worst/best case scenario) without a more extensive OAT analysis involving further assumptions/parameters;
- **Monte Carlo analysis**, where inputs/assumptions are changed simultaneously (i.e. on the basis of the evaluated probability distribution functions expressing the known uncertainty about the inputs).

In a small number of cases, the applied sensitivity analyses cannot be included in any of the proposed classes.

The results with all the details of the analysis should be available for scrutiny, both if quantitative work is performed internally or by a contractor (running the model or the uncertainty/sensitivity study). In addition, the sensitivity analyses could have been performed before and reported in other documents which have to be referred to.

From the IAs exam, it appears that a global approach, which exhaustively explores the input uncertainties to identify the main sources of output uncertainty (as explained in the following pages, see section 4 and 5) is not commonly applied. When SA is carried out, in many IAs, the OAT approach is recurrent and a limited number of assumptions is varied[5].

The real risk of a local analysis is to erroneously estimate the model uncertainty with consequences on the policy evaluation.

It is fundamental to be aware that **SA** is not another step that makes an already complex assessment more difficult. On the contrary, it is a useful (**unique) instrument which enriches the quantitative analysis** of impact with a deeper investigation and identification of the sources of uncertainties.

4 The list of impact assessments carried out in the period 2011-2018 was collected from the European Commission's Better Regulation site. The search was based on the text search of string "Sensitivity analysis", using EUR-Lex. see Becker et al., 2019.

5 The same tendency is evident in Academia. A recent paper shows that many highly-cited papers use the OAT sensitivity analysis rather than the global one (Saltelli et al., 2019).

This implies a serious commitment towards the dissemination of a **SA culture** which contributes to the implementation of better policy making. However, some obstacles which still impede or prevent the performance of (global) SA can be overcome only by continuous engagement and guidance. To achieve a greater 'uncertainty awareness' requires time and effort.

Some **possible obstacles to a wider use of SA** derive from the complexity and/or unknown issue represented by the sensitivity analysis, the lack of specific skills (i.e. technical background), the insufficiency of the resources available (including time), difficulty in finding direct exemplification (such as previous cases), and a reduced control under the quantitative/numerical aspects of the assessment (e.g. when third parties are involved).

Dedicated training and guidelines can contribute to address some of these issues as well as fixing 'incentives' to carry out and report sensitivity analysis as a part of a culture of responsible and quality modelling. For example, it is important to **schedule sensitivity analysis into the workflow** and plan time and resources for it or guarantee transparency about the model and any numerical analysis.

Sensitivity analysis should be covered, at least briefly, in general impact assessment training. Obviously, **policy officers** are not required to become experts in sensitivity analysis, but they should be **supported** in discovering the potential and advantages of the uncertainty and global sensitivity analysis. Whereas interested "advanced practitioners" from policy directorates may be further trained to become an 'inside support' for technical (and maybe specific) aspects of sensitivity analysis in impact assessments within their policy area.

The availability of devoted support and tools to conduct the analysis also plays a crucial role.

The remainder of this report directly aims at further strengthening and supporting the use of UA and SA for impact assessment.

3 Uncertainty analysis

Notwithstanding the unavoidable uncertainty associated with evidence informing policy making, **robust informed decision making** means that **it is possible to infer whether a (policy) option is preferable or not** (see Figure 2). However, at the initial stage, uncertainties might be so high they impede such an informed decision. In this case, knowledge has to be refined as much as possible, by gathering more data to hopefully reduce some of the sources of uncertainty.

In this context, **uncertainty analysis aims to quantify the uncertainty which affects the model information available to the analyst/decision maker**. The resulting uncertainty is theoretically derived from the uncertainties incorporated in the different model inputs[6]/assumptions on which the model outcome itself is based. Therefore, UA starts with identifying and characterizing these sources of uncertainty to infer their impact on measurement-based and model-based evidence. The next steps consist of estimating and shaping the uncertainty under which the decision process has to be made.

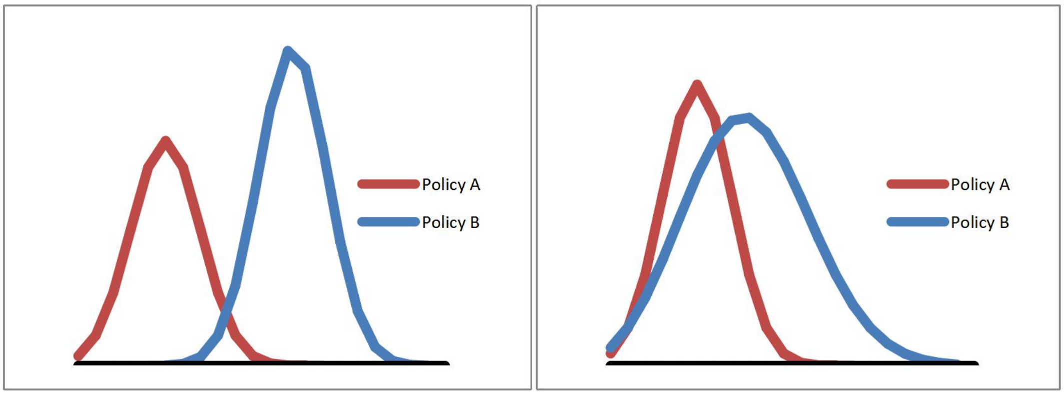


Figure 2. Comparison of the impact of two policies on some given criteria (e.g., cost, GDP, unemployment, …) by accounting for uncertainty. Two outcomes are possible: either a good policy option can be inferred (left), or there is no clear evidence that one policy outperforms the other (right).

The conclusions of **the uncertainty analysis can show that the impact of a policy option is preferable compared to the others.** This means that it is possible to consider the chosen policy as globally better; hence a robust decision can be made. **At the other extreme, the results can also prove that the uncertainties are too large to support a specific choice**. In both cases, the investigation can be profitably integrated by sensitivity analysis (see section 4.2), which can help identifying among the inputs (related to data and/or knowledge) the key sources of model uncertainty responsible for the uncertainty in policy impact.

Thanks to **uncertainty quantification**, the analyst/decision maker is better informed about the nature and relevance of uncertainties. Consequently, possible actions to increase the overall knowledge about policy relevant uncertainties and/or control their effects can be evaluated and implemented.

It has to be underlined that **uncertainty analysis is an iterative process**, that continues either until satisfactory and sensible results are obtained, or the conclusion is reached that,

6 In UA-SA all elements contributing to the model definition (in its widest sense) are generically referred to as inputs.

given the current status of knowledge of the problem, no accurate evidence can be provided (in Box 1 an example of decision making under uncertainty).

The following sections address how to identify the sources of uncertainty (section 3.1) and how to quantify uncertainty in the inputs (section 3.2) and thus in the model response (section 3.3).

Box 1. Decision making under uncertainty.

We consider a model to compute the expected reduction of pollutant concentration (measured in μg/m^3). The model implies several uncertain inputs. For our exercise, all parameters are set to their nominal value. The only input allowed to vary is the '*Policy to be applied*'. Two different policies are compared 'Policy 25%' and 'Policy 100%'.
The UA result is shown in Figure B-1: by applying *Policy 25%* a reduction of the pollutant of about 24 μg/m^3 could be achieved while applying Policy 100% a reduction of about 37 μg/m^3 is expected. Therefore, a difference of 13 μg/m^3 would be achieved if the choice is *Policy 100%*. This inference is of course misleading because it is not clear whether this improvement is significant or not. This is important as *Policy 100%* might be more expensive to apply than the other option. Hence, it is important to assess whether the policy-makers will get their money's worth. One way to ensure that is to account for the modellers' best knowledge about the model input values.

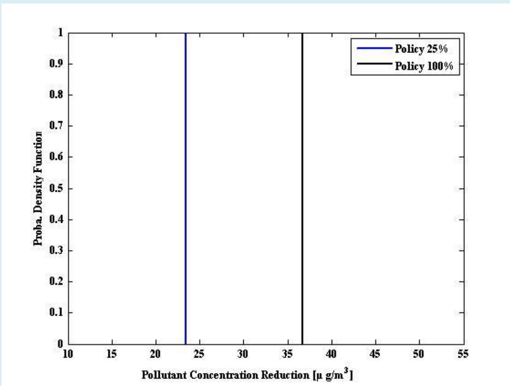


Figure B-1 - Model result assuming model inputs to their nominal value

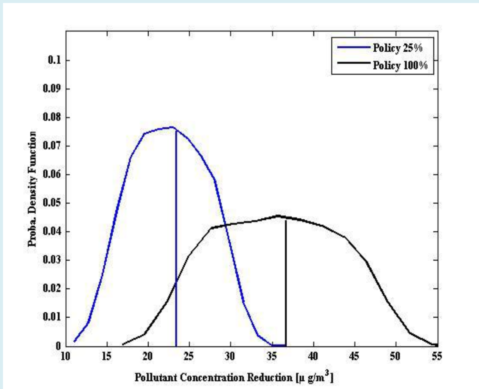


Figure B-2 - Model response when uncertainties in the inputs are accounted for

The model is executed with a random sample in order to account for all uncertain model inputs. The resulting uncertainties in the model responses for the two policy scenarios are depicted in figure B-2. We see that, for the two policy options, the predicted pollutant concentration reduction ranges change and appear characterised by different probability density curves. We also note that the predicted probabilities overlap. In this second case, it is not clear whether *Policy 100%* would effectively be more efficient than *Policy 25%*. In such a situation, it is not possible to make a choice between the two policies. Therefore, it is recommended to identify the inputs responsible for such an overlapping. This is the role of sensitivity analysis.

Source: Adapted from JRC Science for Policy Report - (Albrecht et al., 2018)

3.1 Identifying the sources of uncertainty

There are **several possible sources of uncertainty** which can affect model responses and thus reduce their reliability, effectiveness and quality. Therefore, to ensure a responsible use of model outcomes, uncertainties must be identified and acknowledged. The identification of the sources of variability is the first step to be performed in uncertainty analysis.

Among the sources of uncertainty, we can cite:

– unknown future scenarios;

– parameter uncertainty;
– data errors;
– different opinions (e.g. experts vs stakeholders);
– …

In our declination, UA-SA methods are purely based on input and output analysis without specific consideration of the model peculiarities or the mechanism of uncertainty propagation within the model.

Table 1. Example of input uncertainty quantification.

Label	Parameter	Baseline value	Distribution (1)	Type (2)	Accuracy (3)
X1	Capacity of source N2	31.2	U(16,31.2)	A	L
X2	Capacity of source N19	30.0	U(15,30)	A	L
X3	Capacity of source N10	10.2	U(5,10.2)	A	L
X4	Capacity of source N11	7.0	U(3.5,7)	A	M
X5	Compressor station capacity reduction factor	0.2	N(0.2,0.052)	E	M
X6	Peak demand of Country 1	15.5	N(15.5,0.752)	E	L
X7	Peak demand of Country 2	12.1	N(12.1,0.62)	E	L
X8	Peak demand of Country 3	5.3	N(5.3,0.42)	E	L
X9	Failure frequency of LNG	0.15	N(0.15,0.0152)	E	H

(1) U=Uniform distribution, $N(\mu,\sigma^2)$=Normal distribution of mean μ and variance σ^2 .
(2) E stands for epistemic uncertainty as opposed to A- aleatoric uncertainty.
(3) Modellers belief regarding the assigned prior uncertainty: L=Low, M=Medium and H=High.

The uncertain input variables are reported associated with their baseline values (column #3). These values represent the modellers' best knowledge about these parameters. The uncertainty about these model inputs is acknowledged in column #4. The modellers should indicate whether those uncertainties are reducible (E) or not (A) and their degree of confidence in the values assigned to each input (resp. column #5 and #6).

Source: Adapted from JRC Science for Policy Report - (Mara et al., 2017)

Input uncertainty can be classified as either aleatoric or epistemic. Future scenario uncertainty is typically an instance of aleatoric uncertainty because at the time of its use for model simulations there is no foreseeable way to reduce it further. On the contrary, epistemic uncertainty is supposed to be reducible, provided that more data can be gathered or experiments carried out. Therefore, it is important to classify the different sources of uncertainty before analysing them, and to be prepared to clearly justify the classification made as well as the uncertainty attached to each input. Table 1 provides an example of input uncertainty.

3.2 Quantifying input uncertainty

Once the sources of uncertainties have been identified, the input uncertainties should be characterised. **This critical phase consists of tracing the limits of the known input uncertainties**. Quantifying the uncertainty in model inputs can be demanding. In **worldwide practise**, experts, modellers, stakeholders, and UA-SA practitioners share their knowledge and experience to best display how the investigated model inputs are affected by variability. Other ways to characterize uncertainty are literature review, direct and indirect measurements (i.e. by confronting model responses to observations) or Monte Carlo filtering.

In a probabilistic framework, the input characterization takes the form of joint probability distribution (or probability density function, pdf) associated to each model input. In fact, uncertain inputs are treated as random variables whose perturbations, when propagated into model output(s), will define the output uncertainty.

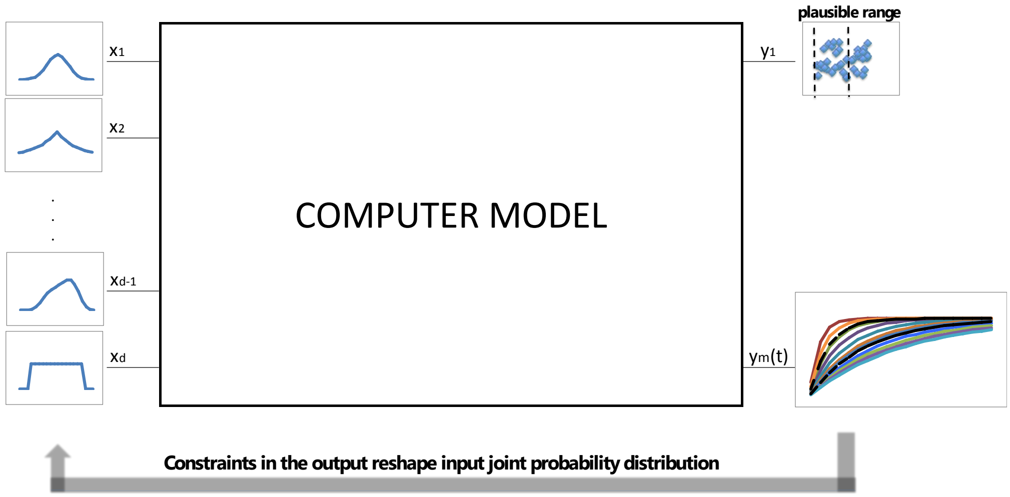


Figure 3. One possible way to shape the joint pdf of the different model inputs (on the left) is to constrain the model responses so as to comply with expert knowledge or some measurement (on the right).

Another strategy to define input uncertainty is to **repeat UA-SA several times during which the input uncertainty is progressively refined**. The analysis may start attributing large pessimistic uncertainty ranges (assuming independent uniform distributions) and performing sensitivity analysis to pinpoint the relevant sources of uncertainty. This initial wide approach usually allows substantial timesaving, as the analyst can identify the key sources of uncertainty and focus specifically on the refinement of the relevant input distributions. The process can be continued until no further refinement is needed or possible. This approach is related to the Monte Carlo filtering (see Annex 3). The Monte Carlo simulations (see Box 2) used to propagate the uncertainty to the model response are split into two categories: i) 'behavioural' and ii) 'non-behavioural' input set of values. By behavioural, it is meant input value combinations that provide sensible model responses (see Figure 3). Consequently, only the behavioural input sets will be taken into account.

All these strategies to define the input (and possibly the output) uncertainty are in line with Leamer (1990) who wrote: "*I have proposed a form of organized sensitivity analysis that I* *call 'global sensitivity analysis' in which a neighborhood of alternative assumptions is selected and the corresponding interval of inferences is identified. Conclusions are judged to be sturdy only if the neighborhood of assumptions is wide enough to be credible and the corresponding interval of inferences is narrow enough to be useful.*"

3.3 Quantifying model response uncertainty

As a further step, after being quantified, **input uncertainties are propagated through the model** up to the response of interest. In this way, also the model output becomes a variable characterised by a specific range and a probability density function that the quantification process aims at shaping. Therefore, as the final step of the analysis, the output uncertainty is characterised (and eventually linked to the level of confidence in the result) and some relevant statistics (such as mean, standard deviation, median) are often inferred.

As previously stressed, the subject of the analysis is the response of interest. Note that it might not be the model output *per se*, but the quantity related to the evidence that are relevant for the decision-makers (Saltelli et al., 2004).

Monte Carlo simulations (Box 2) are very popular approaches to estimate the impact of input uncertainties into model responses because they are model-free (i.e. no specific assumption is required about the model). The Monte Carlo method relies on the generation of a random input set used to run the model. This provides a set of associated model responses from which the output uncertainty can be inferred. We can view a Monte Carlo simulation as a process through which multiple scenarios generate multiple output values (EPA, 2009).

Box 2. Main steps of the Monte Carlo method.

The Monte Carlo method relies on simulated random events. It allows the random propagation of the input uncertainties into the model, in order to cover the overall input space defined by the input uncertainty. In this way, the uncertainty in model predictions can be exhaustively examined and quantified. The Monte Carlo method consists of three fundamental steps:

1. Generate a random input sample of a given size N from the input joint probability distribution (the random sample is also called 'Monte Carlo sample')

2. For each draw of the sample, run the model and save the output(s) of interest

3. Analyse the response sample and characterise its uncertainty

4 From uncertainty to sensitivity analysis

In the previous section, we explained how to quantify the uncertainty in model inputs and how the uncertainty in model output can be assessed by propagating the input uncertainty through the model.

Now, we would like to take it one step further and find out how to **identify what are the main inputs responsible for the model uncertainty**, and measure their individual impact. We could also rank these inputs on the basis of the quantification of their contribution to the output variability. This is precisely the domain of the sensitivity analysis.

We can (loosely) **define sensitivity analysis as** '*the study of how uncertainty in the output of a model (numerical or otherwise) can be apportioned to the different sources of uncertainty in the model inputs'* (Saltelli et al., 2004).

For this reason, from a methodological point of view, we consider that **uncertainty and sensitivity analyses go hand in hand**, with the results of the UA being the starting point of the SA, to such an extent that 'sensitivity analysis' often tacitly incorporates uncertainty analysis.

The **UA moves from the input uncertainties towards the quantification of the output uncertainty**. Once the outcome variability is quantified, the **SA comes back** from this measure to the inputs, quantifying the share of model uncertainty which is due to each factor.

First of all, it is primordial to define the objectives of the sensitivity analysis to be performed. This setting helps clarify the study and also to target the sensitivity indices to be estimated (sensitivity indices are addressed in section 4.3). Some possible sensitivity analysis settings, as already mentioned, are:

- ranking of the inputs by order of importance to prioritize future research (factor prioritisation);
- identifying irrelevant inputs which can be fixed to their nominal values (factor fixing);
- mapping of the input space that provides model responses within some desired ranges (factor mapping);
- investigating what would be the impact on the model response of interest if one or several input variables were changed w.r.t. some base case scenario (what-it-analysis);
- ….

The **'main ingredients' of SA are input and output**. Output is the model result, whereas the inputs are, among the assumptions (scenarios, data, parameters…), those which are allowed to vary in order to study their impact. Therefore, **a relevant part of this analysis depends on our choices**. And a quite obvious consequence of this, is that we will not know about the importance of those assumptions which are kept fixed. For this reason, **an initial accurate analysis design is primordial**. For example, we should evaluate which assumptions to use as an input and their characteristics, such as their range and distribution form, as well as a precise definition of the goal of the study.

With this in mind, it becomes evident why the **SA should not be considered as model-oriented but rather problem-oriented**. This implies that SA does not exhaust its investigation with a one-time model analysis but should be continually carried out every time inputs are modified for the same model and the assumptions/hypothesis of the decision making process are changed.

4.1 Local versus global sensitivity analysis

A number of techniques and strategies are available to carry out the sensitivity analysis, and different formulas can be applied to estimate sensitivity measures (Saltelli et al., 2008; Borgonovo, 2017; Azzini & Rosati, 2019).

Sensitivity analyses were **firstly carried out using local approaches** (Rabitz, 1989; Turanyi, 1990). In local methods, an individual input is changed, while the others are kept fixed, and the resulting outcome is compared with the initial output baseline. Successively, the input may be returned to its initial value and another input is moved. Therefore, the SA examines the variation in the model output by changing the inputs One-At-a-Time (OAT), often between the minimum and maximum among plausible values.

In this kind of approach the input space is explored only around a specific (given) point (the baseline) and the **result can be inaccurate or insufficient in many cases**. Local sensitivity analyses are computationally cheap and rather simple to implement, but they do not account for possible interactions between model inputs or may not be sufficiently informative for non-linear models and/or models with high-dimensional input spaces. Therefore, they **might fail at identifying relevant information** about the impact of model inputs.

A simple illustrative example showing the **possible drawbacks of the One-At-a-Time approach is presented** in the following section.

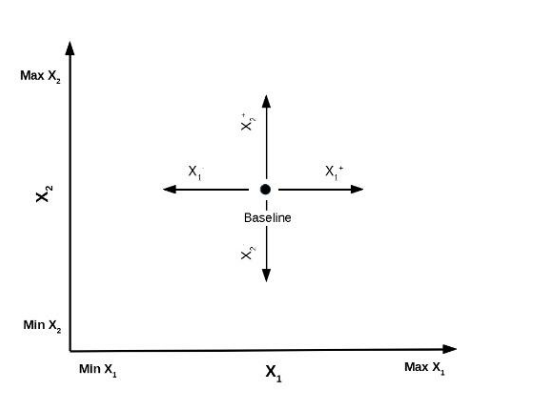
4.1.1 One-At-a-Time – illustrative example

The One-At-a-Time (OAT) method is one of the **most popular approaches** for studying the effect of the model input on the output. Instead of varying simultaneously all the input variables likewise Monte Carlo simulations, **each input is varied in turn w.r.t. the baseline case** (see Box 3). By doing so, it seems easier to infer which input has the highest impact on the model response. Hence, to define the impact of one specific input, we can fix all the inputs at their base-case value (baseline or 'nominal value') except for the investigated input, which is varied within its range. The model is run and, by comparing the model outcomes before and after the change, the variation due to the input is isolated. This variation is the effect given by the moving of the individual input.

This procedure is repeated for all the inputs, continuing to move each element one at a time. In the end, we obtain a picture of the sensitivity of the output to the input variables. The method is usually run referring to the extremes of the input ranges. For example, if input x_1 has its baseline value at 3 and the range is between 0 and 6, the model is evaluated successively for both $x_1 = 0$ and $x_1 = 6$ and the two outputs obtained are compared with the baseline outcome ($x_1 = 3$). A variant is the choice of the best/worse value for the input. The OAT analysis can be more articulated including more points for each input, but always, after the 'perturbation' returning the input to its baseline value.

Box 3. One-At-a-Time (OAT).

One of the simplest and most common approaches to sensitivity analysis is to change one-factor-at-a-time (OFAT or OAT), and observe the output effect. The procedure to perform OAT sensitivity is investigated for each input as follows:



1. *Move the investigated input (ΔX_i) keeping the others fixed at their baseline (nominal) values and measure the new output (compute ΔY_i), then*
2. *Return the input to its nominal value and change each investigated input in the same way.*

Model sensitivity is measured by monitoring changes in the output.

The OAT method has some interesting characteristics:
- any change observed in the output will be assigned with no ambiguity to the single input varied,
- changing one variable at a time, we can keep all other variables fixed to their central or baseline values. This increases the comparison of the results, as all 'effects' are computed with reference to the same baseline;
- sensitivity is measured by $\Delta Y_i/\Delta X_i$.

However, an important drawback of the OAT approach is the fact that it does **not allow to examine varying inputs simultaneously. Sensitivity is dependent on the nominal values.**

Normally, the starting point of an OAT-SA is not just any one of the possible cases, but it often represents the relevant well-known base-case (i.e. baseline). Hence, the interest is in discovering **what happens in the 'neighbourhoods' of this 'preferable' combination** when the inputs change w.r.t. the baseline scenario. In addition, the comparison of the alternative scenarios with the same baseline appears convenient.

Another reason for the frequent application of the **OAT** by modellers/analysts is its **simplicity and straightforward implementation**.

However, despite this simplicity, the approach does not take into account the simultaneous variation of the input variables. In fact, in carrying out the analysis only one input is changed while the others remain fixed, but in reality the inputs can vary simultaneously and some effects can be originated by this concomitant modification of their values. Consequently, this means that the **OAT (by design) cannot detect the presence of possible uncertainties produced by interactions between input variables**.

Therefore, the hypothesis on the basis of the OAT turns out to be quite strong and unrealistic in most cases. This does not mean that the OAT is wrong *per se*, but rather that the method may not be appropriate, and that the approach based on few evaluations of the model is often insufficient and misleading. This results in a perfunctory sensitivity analysis (Saltelli & Annoni, 2010).

Several insights can remain unexplored and the real behaviour of the model is not obtained apart from very specific research questions or regular models (linear and additive) for which the performance in a point is informative of the whole space. Thus, these prerequisites should be verified and carefully justified. Nevertheless, the OAT is very widely used and common in many fields of investigation (Saltelli et al., 2019).

To **illustrate the possible risk inherent to the OAT method** let us look at a very simple example. The model expressing the total cost of our daily shopping is given by:

$$y = \sum x_i p_i$$

where y is the output cost and x_i and p_i are the quantity and unit price respectively of the i goods bought. For the sake of simplicity, if we consider only two products x_1 and x_2, the model becomes:

$$y = p_1 x_1 + p_2 x_2$$

The baseline and range values of each of our four inputs are the following:

	baseline	range
p1	**3**	1-5
x1	**20**	0-40
p2	**1**	1-3
x2	**50**	10-100

Table 2. Model input baseline values and ranges.

so the base-case values assigned to the four factors (p1, x1, p2, and x2) are respectively 3, 20, 1, and 50.

Given these values the model output (total price paid) has a base-case value of 110. Starting from the baseline, we assign 5 to the input p_1. The goal at this point is to test the output response to the variation in the input (line 2 in figure 4). We evaluate the model for this new set of four values. The outcome is 150, with an increase of 40 (figure 4). Then the model is re-evaluated assigning the value of 40 to the quantity x_1, while the price p_1 comes back to 3 (line 3 in figure 4). The output is computed again and compared with the baseline: the difference is 60. A similar procedure is followed for the other two factors p_2 and x_2 (figure 4, lines 4 and 5).

	p1	x1	p2	x2		y	Δy
1	**3**	**20**	**1**	**50**		**110.00**	
2	5	20	1	50		**150.00**	**40.00**
3	3	40	1	50		**170.00**	**60.00**
4	3	20	3	50		**210.00**	**100.00**
5	3	20	1	10		**70.00**	**-40.00**
							160.00
	5	40	3	10		**230.00**	**120.00**

Figure 4. Illustrative example OAT: Baselines are changed and new outputs calculated.

The next step is to evaluate the model when all the four inputs are changed at the same time (last line in figure 4). Finally, the difference between this new model output and the base case is computed.

However, the result is not equal to the sum of the individual variations in the output (when the inputs are changed One-At-a-Time), which is a sign that **something is going wrong**. Specifically, we verify that the increase of the input has produced an increase of 120 instead of the expected value of 160. The difference is due to the effects deriving from the interactions among inputs, which are not captured by the OAT method.

This simple example clearly shows the **risk in deducing the behaviour of the model from the simple evaluation of some specific input changes**, when several other (sometimes infinite) values are possible within their ranges.

We can also note that, when we modify only x_1 and x_2, keeping the prices fixed, the OAT seems to work. This is because the two considered inputs, the quantities, do not interact between themselves and consequently no uncertain effect is generated (see figure 5). Therefore, the sensitivity of these two inputs could be measured by local techniques.

	p1	x1	p2	x2		y	Δy
1	**3**	**20**	**1**	**50**		**110.00**	
3	3	40	1	50		**170.00**	**60.00**
5	3	20	1	10		**70.00**	**-40.00**
							20.00
	3	40	1	10		**130.00**	**20.00**

Figure 5. Illustrative example OAT: Baselines are changed and new outputs are compared.

The use of the **OAT implies the awareness that all the insights about the model hold when one input is changed and all the other factors are kept fixed at the baseline**. This investigative goal must be specified and communicated with the results of the analysis. If the intent of the analysis is to learn about the effects due to interactions (or/and we do not know enough about the linearity of the model) the whole input space must be investigated. In practice, many cases must be taken into consideration. These cases should be obtained by the random combination of possible input values and are able to inform us about the output uncertainty originated by interactions among inputs. A GSA should be applied.

In addition to the original local OAT approaches some more exhaustive global methods have been defined which vary parameters One-At-a-Time but which include i.e. trajectories in the input changes allowing an improved investigation of the model behaviour (see i.e. Morris, 1991; Campolongo et al, 2007; Campolongo et al., 2011; Saltelli et al., 2008).

Moreover, during the last few decades, the remarkable methodological development, which has characterized the SA domain, provides highly-efficient methods of investigation and permits a drastic reduction of the computational time (which was one of the serious limits of a more extensive analysis). Consequently, **global sensitivity approaches**, traditionally unaffordable, are today effortlessly (or with greater ease) carried out. Therefore, they **are recommended and preferable** (Sudret, 2008; Shao et al. 2015; Saltelli et al., 2010, Azzini et al., 2020).

4.2 Global sensitivity analysis methods

The **global approach was introduced in the early nineties** and, since then, it has been widely applied (i.e. Medicine, Environment, Engineering, Chemistry …), playing a **key role in modelling**. A 'global' approach for quantifying uncertainty allows for the simultaneous and full range exploration of all sources of known uncertainty. Most of the global approaches are compatible with the Monte Carlo simulations discussed in section 3.3 and therefore they allow a simultaneous execution of both uncertainty and sensitivity analysis.

Global sensitivity analysis (GSA) overcomes the drawbacks of local analysis and it is able to highlight the uncertainty effects originated by interactions among model inputs, whatever the dimension. This kind of exhaustive analysis is strongly recommended when models are not linear (Campolongo & Saltelli, 1997, Saltelli & Annoni, 2010), and better assures against the risk of discarding an input that is actually important. Global sensitivity analysis can also be designed to address the impact of different model choices.

Among the most relevant GSA techniques, we find screening methods (Morris, 1991, Campolongo et al., 2011), non-parametric or regression-based approaches (Saltelli & Marivoet, 1990; Helton, 1993), variance-based methods (Sobol', 1993; Saltelli et al., 2008; Iman & Hora, 1990; Sacks et al., 1989) and the spectral methods (Cukier et al., 1973; Saltelli et al., 1999; Sudret, 2008; Shao et al., 2017), and moment-independent importance measures (Park & Ahn, 1994; Plischke et al., 2013).

In particular, **variance-based methods related to Sobol' sensitivity indices are the most popular methods among GSA practitioners** due to their versatility and easiness of interpretation. In this framework, the output uncertainty is measured by the total variance that can be decomposed into partial variance contributions of increasing dimensionality. In more simple words, the model uncertainty is defined as the sum of uncertain effects due to individual or interacting inputs.

This decomposition was introduced by Hoeffding (1948), while Efron & Stein (1981) showed its uniqueness. Subsequently, Sobol' (1993) decomposed the total variance of model output into additive terms, which represent the sensitivity effects, in a unique way and proposed the so-called sensitivity indices as uncertainty measures. Sobol' indices represent the amount of the total output uncertainty due to each inputs, solely or by interaction with the others.

Sobol' sensitivity indices can be estimated exclusively from input and output values. Therefore, variance-based methods are **model independent** (albeit some mild assumptions), which makes them **particularly versatile**. In some cases, they can be also applied to the analysis of groups of inputs. If correctly built, **the same sample already used for the UA can be the starting point of the SA.**

Several computational methods aim at the estimation of the Sobol' indices such as sampling-based Monte Carlo approaches (Saltelli et al., 2010; Saltelli A., 2002; Sobol', 1993), spectral approaches (Saltelli et al., 1999; Cukier et al., 1973; Sudret, 2008; Shao et al., 2017) or metamodeling-based approaches (Oakley & O'Hagan, 2004; Buzzard & Xiu, 2011).

In the following of the present work, due to their relevance, we will focus on variance-based methods and Sobol' sensitivity indices.

4.2.1 Implementation steps

Uncertainty and sensitivity analyses imply a careful planning during the model design and execution for impact assessment. Throughout the UA–SA process, modellers/analysts, experts, and stakeholders must constantly engage with the SA. In this way, the relevant elements of the model can be identified and the data necessary to conduct the analysis provided. In addition, the SA results can be correctly interpreted and linked to their concrete meanings in the real world.

The **basic steps to perform GSA** are the following:

1) **The model output of interest must be clearly identified**.
   Define the model output of interest for the analysis. During this first phase, the goal of the analysis and the relevant model output(s) should be clearly defined. The latter consists in (or is related to) the outcomes which are of more concern to the impact assessment (e.g. GDP, pollution abatement, unemployment reduction, energy consumption or saving…).

2) **All sources of the uncertainty must be listed and possibly classified.**
   Identify all model inputs that are affected by uncertainty and can potentially have an impact on model output of interest. In this crucial phase, the analysts, with different contributions from e.g. experts, stakeholders, and UA-SA practitioners, identify which inputs/assumptions should be considered as relevant to the study. Only these relevant elements will be considered in uncertainty/sensitivity analysis. These inputs can be of various nature (i.e. scenarios, data, parameters, model, choices) and of various types (i.e. scalar, time series and/or spatially distributed, scenarios, maps).

3) **The objective of the GSA must be defined and the most adequate method chosen.**
   Define what is the objective of the sensitivity analysis which points to the sensitivity indices of interest. Then, choose the method to apply by balancing the trade-off between accuracy of the estimation of the sensitivity indices and the computational burden.

4) **The uncertainties in the input must be quantified and justified.**
   Characterise the uncertainty for each selected input. Each uncertain input is characterised by assigning a range of uncertainty (ex.: a statistical distribution or a probabilistic density function) and possible associated with a correlation structure. This can be inferred from all the available information such as experimental results, estimations, physical bounds, and experts and stakeholders' opinions as well as peer reviewed references.

5) **A random sample is generated allowing the full investigation of the input space**.
   A sample with the desired characteristics established during the previous phase, and related to the chosen GSA method defined in 3) is generated. The sample size corresponding to the number of model runs should be chosen by taking into account the computational time of the model ad also the desired sensitivity methods to be employed. Practically, the sample could be considered as a matrix in which each row identifies a specific set of input values that we need to run the model. The random generation of a sample can be easily obtained through software packages (today they are largely available also in free-versions).

6) **Input and output must be traced**.
   Run the model for each draw of the random sample and save the model response of interest. We recall that the latter should be related to the relevant outcomes for the impact assessment. For the following analysis, it is primordial to be able to trace how the model output has been produced and which are the input assignments 'responsible' for each model outcome. For this reason, it is essential to link each input set to the corresponding output which must be carefully recorded.

Note that **the steps described above are common to both uncertainty and sensitivity analysis**. At this point, the uncertainty in the model response of interest can be quantified (see previous section about uncertainty).

7) **The different statistics for UA-SA are inferred.**
   With the input-output data obtained from 6), the analyst can infer the relevant statistics for the uncertainty and sensitivity analyses. For the sensitivity analysis, these statistics are called sensitivity indices (these are discussed in section 4.3).

8) **UA-SA results are reported in a comprehensive way**.
   Report the conclusions/inferences in a sensible and comprehensive way, taking into account the goal of the analysis and the background of the addressee of the analysis (i.e. modellers, policy-makers, experts, and stakeholders). Sensitivity results can be reported in the form of a chart or a number (indicator) representing the importance of the key variables for the quantity of interest. Uncertainty in the output could be represented by e.g. ranges of variation or histograms.

9) **UA-SA is a recursive process which can be repeated until a satisfactory solution is found**.
   The results may require a deeper analysis. The involved parties can agree with a further investigation. UA-SA can be re-run on the basis of a refining in model assumptions.

Sensitivity analysis might be demanding in terms of time and human resources, consequently a timely evaluation of its cost and feasibility is primordial. However, research in the SA field has made available software which can carry out investigations and computations which were still unimaginable only a few years ago.

Sensitivity analysis is a mature discipline whose complexity has significantly increased in the recent past, **advanced but easy-to-use tools can provide support** thanks to these theoretical development and methodological improvements.

Besides, when used for policy making, the **cost of carrying out UA-SA should be compared with the risk of the consequences of an incomplete analysis (i.e. selecting a wrong policy option)**, this especially considering that they could have an impact at the EU level. Above all, reliable and credible models are of paramount importance for evidence based policy making.

4.2.2 Main limitations and difficulties

Some common pitfalls and difficulties in sensitivity analysis include:

Missing/insufficient information. As we stressed in points 2) and 3) above, the sensitivity analysis of model output critically depends on input uncertainties and the initial ability of identifying/characterising all the input sources of uncertainty to be investigated. The information about the probability distributions and/or ranges of some model inputs is not available (unknown). Alternative strategies must be applied to derive this missing knowledge such as experts' opinions, consultation of previous analysis, peer-review literature… A technical solution is to assign very large ranges and/or standard pdf (typically a uniform distribution) to each undefined input and then progressively refine the analysis on the basis of the intermediate outcomes. Obviously, in this phase a key role is played by the modellers/analysts' experience.

Input dependence. The goal of the sensitivity investigation is to link the output uncertainty to each investigated input. This implies that the effect of each input/assumption should be clearly limited. Therefore, the existence of possible dependency or correlations between inputs must be handled with extreme caution. In general, sensitivity methods assume independence among inputs. When this condition is not verified, some critical precautions must be taken under the risk of invalidating the entire outcome of the SA. Although some methodologies have been defined (Li & Rabitz, 2010; Mara & Tarantola, 2012; Tarantola & Mara, 2017), the management of correlated inputs is still a crucial and open issue today.

Model interactions. A completely different issue is to cope with non-linear and/or non-additive models where the final input effect on the model output also depends on the effect of other model inputs. Global sensitivity analysis of model output easily deals with this apparent problem referring exclusively to input/output uncertainties. At the same time, to consider the model as a 'black-box' does not allow any further speculation about the uncertainty propagation. If the model is very simple and does not present these kind of constraints (the model is linear and additive), easier SA method might be applied as the One-At-a-Time (OAT) method. If not, a partial sensitivity analysis can deliver poor results and i.e. possible interactions among inputs are not detected or relevant elements are not identified. Nevertheless, these kinds of practices are still widely applied.

Computational time. As mentioned in point 6), the sensitivity analysis is based on random model outcomes. This often implies to run the model under investigation several times. Due to the complexity of models, a common and significant problem is the cost of this investigative step in terms of computational time. A single run of the model can take a significant amount of time (minutes, hours or longer). In addition, when the number of uncertain inputs is large, the multidimensional input space to be explored by the SA grows in size. Consequently, also the number of runs and the required time increase. As stressed, a timely analysis design and an adequate choice of the SA are essential. Unfortunately, the computational time is still a problem in several domains.

Combination of various simulation models. Finally, a difficulty that one may encounter in practice is when several models are used in cascade. For instance when models of energy, water, food, land and climate are interlinked. In this case, the outputs of some models become the inputs of others and can even loop. Performing UA-SA of such interconnected models is challenging but still feasible if the necessary resources, including time, are available. A possible approach would be to perform the UA-SA of each model separately as a first step and then to perform the UA-SA of the interlinked model by focusing on the relevant sources of uncertainty previously identified.

4.3 Sensitivity indices

Performing sensitivity analysis of model output requires the definition **what is meant by "important" input**. This is usually defined mathematically by using indices. There are several sensitivity indices that one can rely on which can be classified as,

- importance measure for screening purposes (e.g., Morris, 1991);
- variance-based importance measure (Sobol', 1993);
- density-based importance measure (Borgonovo, 2007).

The first one are qualitative importance measures. They are usually computationally cheap to estimate (i.e., the number of model runs required is rather small) and are relevant to address "factor fixing setting" (i.e., identifying the irrelevant inputs) in the context of high-dimensional model (meaning that the number of input variables is high).

The last two sensitivity indices are instead quantitative importance measures. Their value ranges within [0,1]; the higher the sensitivity index the more important the input variable. They are model-free in the sense that they can be applied to any model irrespective of its complexity.

Variance-based sensitivity indices were introduced by the Russian mathematician Ilya Sobol', who introduced the concept at the beginning of the nineties, marking a turning point in the SA field (Sobol', 1993, Homma & Saltelli, 1996). These sensitivity indices are also called **Sobol' indices**. It is assumed that the overall model output uncertainty is captured by its variance (a second-order moment of the random variable). In effect, Sobol' showed that the output variance can be decomposed in a unique way into the sum of a finite number of partial variances provided that the inputs are **independent** of each other. The partial variances represent different contributions of the input variables (sole or mutual cooperative contributions, see Box 4). Sobol' sensitivity indices can be used to address different GSA settings as explained in Saltelli et al. (2004).

Density-based importance measures (e.g. Borgonovo, 2007) do not rely on any specific statistical moment of the model output (like the variance). On the contrary, they are based on the discrepancy between the unconditional probability distribution of the model output and the conditional probability distributions of the model output obtained by fixing the value of one or more input variables. With such importance measures, it is possible to address several GSA settings.

There are several methods proposed in the literature to estimate these sensitivity indices. Some are computationally demanding while others are cheaper. **We recommend whenever possible to use methods that allow us to properly address simultaneously UA and SA**. These methods usually require one single set of Monte Carlo simulations, the size of which depends on the context (number of inputs, GSA setting addressed, running time of the model, etc.) and the desired accuracy of the calculations. However, sometimes they may fail on the first round and need extra model runs.

Therefore, taking this into account, SA practitioners will choose one of these sensitivity indices and possibly several of them. Indeed, **it is common practice when the number of model inputs is high to first use a screening method (computationally cheap) and then a quantitative method**.

4.3.1 Sobol' sensitivity indices

As **SA results might play a key role within the decision making process,** we would like that **they are easy to understand for the users** i.e. a measure in a compact format such as a number: a unique, simple number linking the input and output uncertainties. This measure should be obtained in a **fast and standard** way i.e model free, in the sense that we can conduct the analysis simply on the basis of the input and output, without any other conditioning from the model complexity. In addition, we would like to get the SA directly from the same Monte Carlo sample we use for the UA without having to do more model evaluations, resulting in more costs in terms of resources and time. Finally, these results must be **easy to communicate** and shareable.

The variance-based Sobol' sensitivity indices are such measures.

Sobol' sensitivity indices are the **most popular importance measure**. In simple terms, as discussed before, in a variance-based context, the uncertainty of the model is measured by the global effect of the model variance. In turn, this model variance is caused by the individual input uncertainties. Consequently, **we can decompose the global effect (model uncertainty) with respect to each investigated input**. The input effects are then translated into indices giving the sensitivity indices (Box 4).
For the purpose of the present discussion, **two Sobol' indices** of the input x_i are to be considered as a reference: **the first-order index S_i and the total-order index ST_i**.

The first-order sensitivity index, also called **main effect index**, is defined as the part of the model variance that is **caused by one input alone** (input that we generically indicate with x_i). The Sobol' main index of an input refers to the effect individually produced by the input and it is expressed as a simple percentage of the variance.

Box 4. Sobol' sensitivity indices.

Sobol' indices are inferred from the decomposition of the model output total variance (denoted *V*). By considering the case of three inputs, we distinguish seven different effects:

$$V = V_{x_1} + V_{x_2} + V_{x_3} + V_{x_1,x_2} + V_{x_1,x_3} + V_{x_2,x_3} + V_{x_1,x_2,x_3}$$

3 first-order effects: direct effect of the input

3 second-order effects: the variances given by the pair interactions

1 third-order effect: the effect given by the interaction of the three inputs.

By dividing by the total variances (V), we obtain the Sobol' indices:

$$1 = S_{x_1} + S_{x_2} + S_{x_3} + S_{x_1,x_2} + S_{x_1,x_3} + S_{x_2,x_3} + S_{x_1,x_2,x_3}$$

The total-order sensitivity index of the input x_i is given by the sum of all the indices including the input:

$$ST_{x_1} = S_{x_1} + S_{x_1,x_2} + S_{x_1,x_3} + S_{x_1,x_2,x_3}$$

Main properties of variance-based sensitivity indices

$1 \geq ST_{x_i} \geq S_{x_i} \geq 0$	Always when inputs are independent
$\sum_{i=1}^{d} S_{x_i} \leq 1$	Always when inputs are independent
$\sum_{i=1}^{d} S_{x_i} = 1$	Additive model (no interaction)
$1 - \sum_{i=1}^{d} S_{x_i} \ll 0$	Indicator of the presence of interactions – The total effect of x_i is not fully explained by its main effect

- d is the number of inputs.

If the entire uncertainty of the investigated model/process is considered equal to 1 (see Box 4), the main effect index will have a value between 0 and 1, because it is a portion of the total model variability. This sensitivity index is 0 when the input has no effect, meaning that there is no direct impact on the model uncertainty. On the contrary, the main effect index is 1 when the input alone is responsible for the entire variability. Obviously, the sum of the individual first-order indices of all inputs cannot be higher than 1 (which expresses the total uncertainty of the model).

When a part of the final uncertainty comes from the common action of two or more inputs, we have to consider the interactions among them. As we explained, to express this additional effect, we need the total-order sensitivity index (Homma & Saltelli, 1996, Saltelli et al., 2010).

The total-order sensitivity index accounts for the total contribution to the model variability due to the input x_i. This index refers to the first-order effect of the input (direct contribution) plus all the other effects (uncertainties) that derive from the **possible interactions between the input x_i and the other model inputs**. Consequently, for definition, the total-order index includes the main index: the total-order index is always greater or equal to the first-order index. **The total-order sensitivity index** is still lower than 1 or equal to 1 but, in the case of interactions (i.e. $ST_i > S_i$), the sum of all these indices **is greater than 1** (the sum is equal to 1 if there is no interaction). This is because each contribution deriving from interactions involves at least two inputs, so it appears more times depending on the number of factors involved. Therefore, the interaction effect contributes to all the total-order indices of the interacting inputs.

The Sobol' sensitivity indices are simple numbers linking the input and output uncertainties and their interpretation is quite easy and straightforward, in fact, being ratio of the variance, they are dimensionless. This gives a great generality to the SA conclusions and **allows immediate comparison** between results from different sources. For example if the main effect index of the input is 0.05, the factor alone explains 5% of the model uncertainty.

Table 3. Sobol' Sensitivity Index – advantages and drawbacks.

Advantages	Drawbacks
- Reliable - Model-independent - Complete picture - UA & SA simultaneously - Easy to use - User-friendly - Broad-spectrum - Easy to communicate	- Not easy to explain mathematically - Can be computationally demanding - Assume independence of the inputs

Finally, the intrinsic simplicity of these sensitivity indicators allows their **effective communication and sharing**. Therefore, if we can decompose the model variance as just explained, we would have a powerful tool to support the policy decision making (Table 3).

However, the variance decomposition assessment can be a complex and challenging exercise.

The CC-MOD SAMO team studies the way to solve this issue and to offer adequate and effective evidence to support transparency and quality in model use.

The activities of the CC-MOD SAMO group provide specific support in this respect, directly contributing to transparency and quality in model use and thus sound evidence for policy support.

In particular, **the Competence Centre on Modelling has recently developed an online tool for EC staff to carry out UA-SA** and to obtain the needed sensitivity indices in a **quick and practical** manner. The functioning of this WebApp, including a practical example, is explained in the section 5. Its main functions are described in detail in Annex 1.

5 The online CC-MOD WebApp for sensitivity indices estimate

In order to assist the European Commission staff, especially in connection with impact assessment activities, the Sensitivity Analysis of Model Output (SAMO) team of the Commission **Competence Centre in Modelling (CC-MOD,** within Directorate JRC.I Competences), **has developed an online application**, available to Commission staff at https://web.jrc.ec.europa.eu/rapps/sensitivity/ (Commission internal link).

This tool allows modelers/analysts working within the Commission **to carry out variance-based GSA and compute the Sobol' sensitivity indices** (Sobol', 1993) **in a practical and user-friendly way** from a given Monte Carlo dataset.

The **functioning of the WebApp is described in Annex 1**.

The CC-MOD WebApp computes the Sobol' indices with the Bayesian sparse polynomial chaos expansion (BSPCE, Shao et al., 2017 – see Annex 2).

No specific quantitative background is needed **to run the SA-WebApp**. The user must however be familiar with Sobol' sensitivity index concepts and have a generic understanding of their interpretation (see previous sections).

Concretely, the dataset to be provided to the WebApp must include N independent set of input values (input random sample **X**), which are used to execute the model, and the associated model responses **y**. The input/output dataset [**X**,**y**] must be stored in a file, with the vector of model responses in the last column. The file should have a 'csv' format - or any other ASCII extension like 'txt' - where data are hold with a specific separator (comma, semi-column, tabulation). It is not mandatory, but in the first row of the file the input names can be indicated (e.g. $x_1;x_2;\ldots;x_d;y$). These labels are recognized by the tool and used to identify the different inputs.

If data are successfully uploaded, the program can be executed, otherwise a warning message is displayed. Once the calculation is achieved another message appears to notify the end of the calculation to the user.

The WebApp provides different types of results, for example:

- The uncertain distribution of the output response together with a table of the relating main statistics;
- Sobol' indices of each variable;
- The joint effect (i.e. interactions) of the inputs;
- The marginal effect of each input versus the output response (scatterplots). The marginal effect normally shows the trend of the effect of each variable onto the model response y.

The WebApp results can be downloaded in '*csv*' format (the file will include microdata) and all the tables/figures proposed can be copied and/or saved. Annex 1 includes a short manual of the WebApp. An illustrative example of SA is given in the section 5.1. Results, main tables, and figures have been obtained using the CC-MOD WebApp.

5.1 Sensitivity analysis of model output – illustrative example

Let us consider as an illustrative example a six input model. As we explained, we do not need to know about the model function in order to carry out the variance-based GSA. What we need is only information about the model input and the corresponding output.

The probability density functions of the six uncertain inputs are assumed to be uniform and their ranges of variability are shown in table 4.

Table 4. Model Input values and ranges.

Input	Min	Max	pdf	Type	Accuracy
x1	1	2	U	C	H
x2	0.2	10	U	C	L
x3	205	235	U	C	L
x4	0	100	U	C	M
x5	9.5	10.5	U	C	M
x6	[0-1-2-3]		U	D	H

(1) U: Uniform distribution
(2) C: Continuous variable, D: Discrete variable
(3) Modellers' belief regarding the assigned prior uncertainty: L=Low, M=Medium and H=High.

The ranges of variability of the relevant inputs, limited by the minimum and maximum value of the input, together with their probability density function (pdf) are used for the **random generation of an input sample** composed of 200 elements (where each sample element is constituted by 6 input values). The associated 200 output values are obtained by running the model using this random sample (table 5 gives an example of I/O of the sample).

x1	x2	x3	x4	x5	x6	output
1.5	5.25	220.65	50	10.07	1	105059.5
1.25	2.88	226.9	35	10.11	2	91786.49
1.75	7.62	214.4	65	10.04	0	126519.4
1.88	6.44	211.28	72.5	10.12	2	140911
1.38	1.69	223.78	42.5	10.05	0	89658.99
1.62	8.81	230.03	57.5	10.02	1	119189.7
1.12	4.06	217.53	27.5	10.09	3	86499.48
1.69	2.28	209.71	31.25	10.06	3	93660.18
1.19	7.03	222.21	61.25	10.13	1	120414.9
1.94	4.66	228.46	46.25	10.1	0	111961.5

Table 5. Model I/O file structure.

Starting from this I/O file, a GSA is performed computing the Sobol' sensitivity indices as described in the previous sections.

The **UA** provides the following statistics **for the model output**:

Mean	Std.Dev	Median	Min	Max	95% CI
106052.8	15739.8	102728.3	79192.66	153557.8	[83531.32,143998.76]

Table 6. UA- Output main statistics.

We obtain (see table 6), that the model output has an average value of about 106,000, with a modest standard deviation of 15,700. The minimum and maximum values are 79,192 and 153,558 respectively. The confidence interval (95%) is between 83,531 and 143,999. In figure 6, a graphical representation of the **distribution of the model output** value is proposed in the form of a histogram and the estimated model pdf is added.

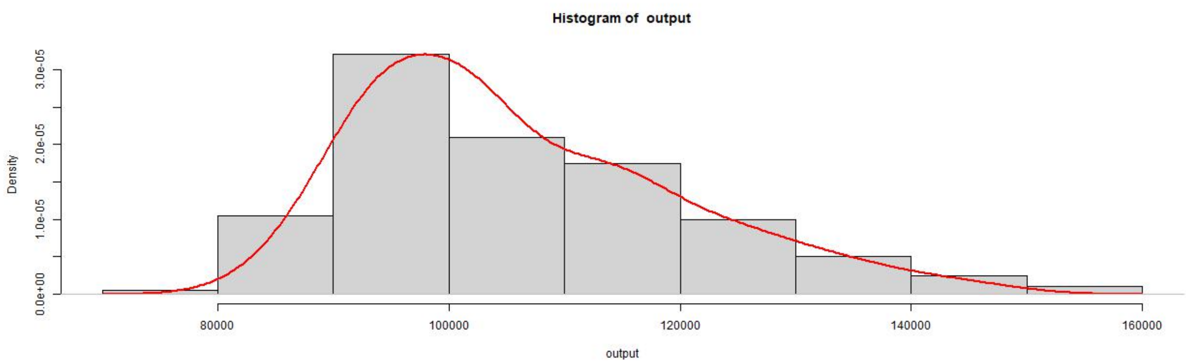


Figure 6. Output uncertainty probability estimate versus its histogram. Source WebApp calculations.

The **SA results** are reported in table 7, where S indicates the first-order index and ST the total-order index (see section 4.3.1). They show that **most of the model uncertainty is explained by the direct effect of only two inputs**: variable 2 and variable 4 which show significant first-order index (0.28 and 0.47 respectively). A further main effect is produced by the first input (0.10), while for input x3 and x6 the first-order index is zero.

A small interaction is detected between x2 and x4. These two inputs have a total-order index higher than their first-order index (0.37 and 0.28 for input x2 - 0.57 and 0.47 for x4), which means that a part of the final model effect is given by the interactions among inputs. The total-order sensitivity indices of x3 and x6 are both zero denoting a complete insignificance of the two inputs in terms of uncertainty. This means that, in this example, the analysists can focus their attention on the other variables.

Input	S	ST
x1	0.1	0.1
x2	0.28	0.37
x3	0	0
x4	0.48	0.57
x5	0.04	0.04
x6	0	0

Table 7. Sobol' indices (S: first-order index; ST: total-order index).

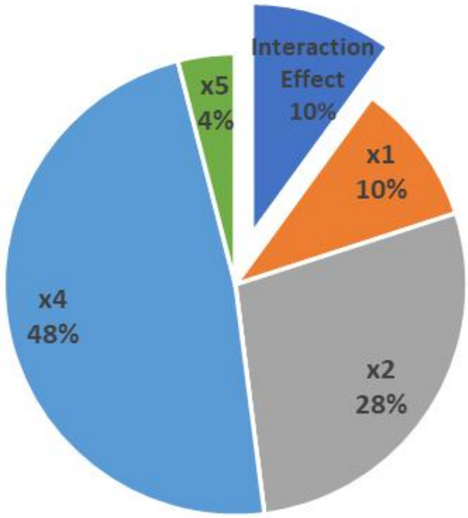


Figure 7. Sobol' indices in the form of a pie chart.

In figure 7, **the entire model variance is represented as a pie chart** and the different sources of uncertainty have been highlighted. The main indices of the significant inputs have been reported and the total-order effect has been emphasized: 10% of the model uncertainty depends on the interaction effect of x2 and x4 (see table 6: the sum of first-order indices is around 0.90).

For each investigated input, **Sobol' main effect and total-order indices can be presented in a graph** as in figure 8 where in red the main effect is plotted and in blue the total effect. The distance between the red and blue points represents the uncertain effect given by the interaction between the variable and other inputs.

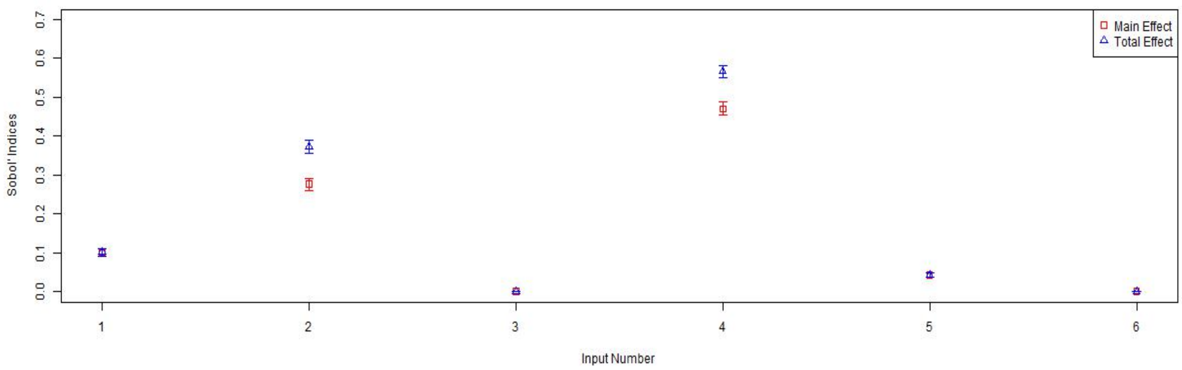


Figure 8. The sensitivity indices results. First-order vs Total-order effects. Source: WebApp.

In addition, some **very useful representations of the relationship between I/O** are the scatterplots (for details see also Annex 3). Figure 9 shows the scatterplots of the output dataset versus one relevant input (x2 first plot) and versus the irrelevant input x6 (second plot). The linear regression line has been added to the graphs and is shown in red. A significant slope of this curve is a sign of the direct effect of the input. Both main and total-order indices of the variable are provided in a box within each plot.

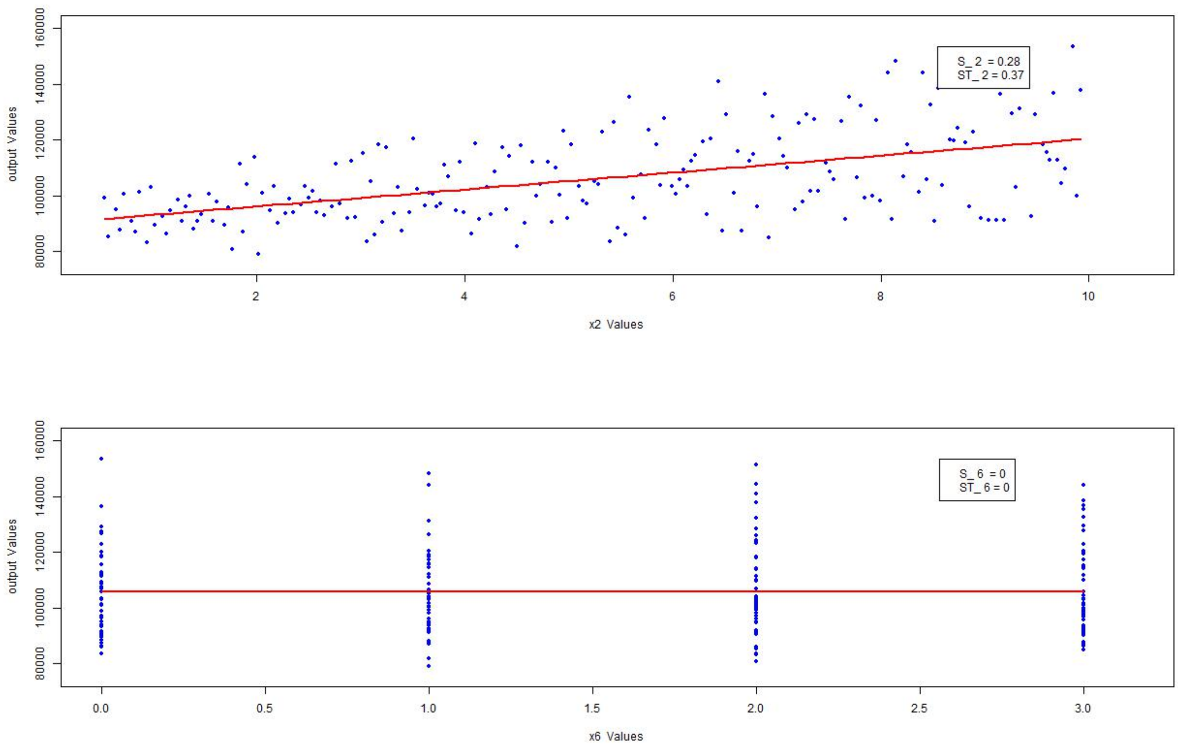


Figure 9. Scatterplots of output versus the input datasets. The red curve captures the trend of the I/O relationship. Note that when the input is non important the curve is completely flat (bottom). Source: WebApp.

6 Conclusion

Simulation models are simplified representations of reality that are developed and used to study the behaviour of natural and artificial systems. Models can also provide support to policy makers throughout the policy cycle and across a wide range of policy areas, and are increasingly used for assessing the impact of policies. **Sound and transparent model use is vital to the delivery of high quality, policy relevant results**.

Model outcomes are inherently affected by a certain degree of uncertainty, which in many cases can be very significant. Responsible model use for policy support requires accounting for the different sources of uncertainty related to the model. Hence, these should be identified and quantified to the extent possible, as indeed the quantification of uncertainty of model results can **affect the decision makers' choices**.

Acknowledging and quantifying uncertainty is a complex and multi-faceted issue. **Uncertainty analysis (UA) and sensitivity analysis (SA)** play an important role among the available methodologies, and **are an integral part of the modelling process**. Nowadays, they are mature disciplines, well-established and employed worldwide in different fields of investigation.

While uncertainty analysis (UA) aims at quantifying the uncertainty in model output due to the uncertainty in model inputs, sensitivity analysis (SA) identifies which are the important sources of uncertainty in the model inputs. This is crucial as the sources of uncertainty can affect the model response. This implies that **modellers** must pay a lot of attention to the latter and characterise them with caution. Whereas, **policy makers** must be aware of the uncertainty in the model response and of the main uncertainty sources, as this can possibly affect their final choice.

In the present report, we have tried to **highlight the added value given by performing UA-SA in modelling activities and IAs**. At the same time, we present some of the **caveats**, limitations and pitfalls that should be avoided when performing such analyses.

Modellers and DGs in charge of impact assessment are encouraged **to ensure that UA and SA are systematically performed in modelling activities in support of policy making**. They should be proportionate to the impact and complexity of the model, and carried out both when models are run by Commission services and by external contractors.

In this respect, the Competence Centre on Modelling **(CC-MOD) has developed an online application** that provides some useful statistics for UA-SA purposes, which has been presented briefly. Further information and support can be obtained by directly contacting CC-MOD.

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List of abbreviations and definitions

CC-MOD	Competence Centre on Modelling
CoP	Community of Practice on Modelling
DGs	Directorate Generals (DGs) of the European Commission
IA	Impact Assessment
GSA	Global Sensitivity Analysis
MC	Monte Carlo
MIDAS	Modelling Inventory and Knowledge Management System of the European Commission
MQA	Model Quality Assurance
OAT	One-At-a-Time
PCE	Polynomial Chaos Expansion
SA	Sensitivity Analysis
SAMO	Sensitivity Analysis of Model Output
S_i	Sensitivity First-order Index
ST_i	Sensitivity Total-order Index
UA	Uncertainty Analysis

List of boxes

List of figures

List of tables

Annexes

Annex 1. An EC WebApp for sensitivity analysis – USER GUIDE

The Sensitivity Analysis of Model Output (SAMO) team of the Commission Competence Centre on Modelling (CC-MOD) has developed an online application to allow any modeller/analyst within the Commission to compute variance-based sensitivity indices, also called Sobol' indices (Sobol', 1993), in a practical and user-friendly way.

The WebApp for sensitivity analysis is available to Commission staff at https://web.jrc.ec.europa.eu/rapps/sensitivity/ (Commission internal link).

Uploaded file structure. To use the WebApp the modeller should first drawn N independent random sets of the d model inputs (matrix **X**). For each draw the model should be executed and the corresponding output scalar response y = $f(x_1,\ldots,x_d)$ evaluated. Hence, the modeller has a Monte Carlo sample [**X,y**] at hand, of the form:

$$\mathbf{X}=\begin{bmatrix} X_{11} & \cdots & X_{1d} \\ \vdots & \ddots & \vdots \\ X_{N1} & \cdots & X_{Nd} \end{bmatrix} \text{ and } \mathbf{Y} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_N \end{bmatrix}$$

where each row corresponds to the I/O of a model run.

THREE SIMPLE STEPS to carry out UA-SA with the CC-MOD WebApp

Step 1: **Uploading data**

Step 2: **Execution of the program**

Step 3: **Analysis of the UA-SA results**

Requirements: To run the WebApp a file [**X,y**] including the uncertain input values and the corresponding output is needed. The first columns of the array should contain the Monte Carlo input sample [**X**], the last column the corresponding values of the model response **y**.

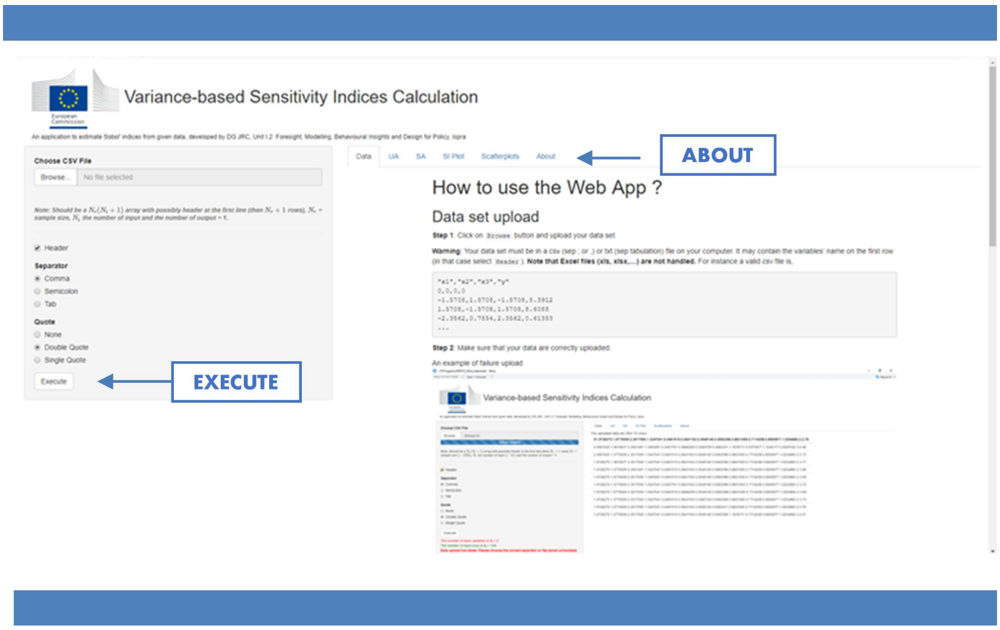
X1	X2	X3	X4	X5	X6	y
1	5.25	1.5	220.65	10.07	50	105059.5
2	2.875	1.25	226.9	10.105	35	91786.49
0	7.625	1.75	214.4	10.035	65	126519.4
2	6.4375	1.875	211.275	10.1225	72.5	140911
0	1.6875	1.375	223.775	10.0525	42.5	89658.99
1	8.8125	1.625	230.025	10.0175	57.5	119189.7
3	4.0625	1.125	217.525	10.0875	27.5	86499.48
		…	…	….	….	

Step 1: Uploading data

1. The WebApp is available at https://web.jrc.ec.europa.eu/rapps/sensitivity/. After clicking the link, the User is connected to the application and the **WELCOME PAGE** is opened. The welcome page is depicted in Figure A1-1. On the right-hand side, a short guide about the WebApp usage is available. Further information about the applied SA method is given in Tab ABOUT.

2. On the left-hand side, click the **Browse** button to select the file to upload from your computer. The file must have a 'csv' format, or any ASCII format like 'txt', where data are saved with a specific separator (comma, semi-column, tabulation). It is not mandatory but the first row should contain the name of the variables (e.g. x1;x2;….;xd;y). This name is recognized by the tool and used to identify variables when displayed. **Note that Excel files (xls, xlsx,…) are not handled.**

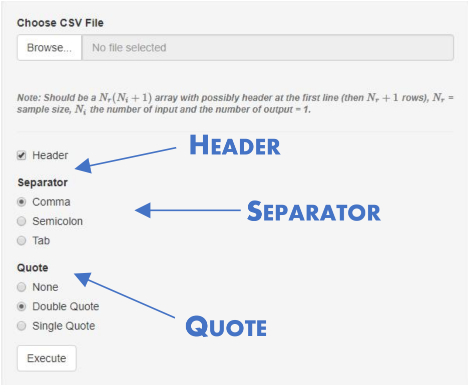
Figure A1-1
Welcome page



3. Select or unselect **Header**. If the file contains the variable names in the first row the field must be selected otherwise the labels are considered as data and the upload fails when executed.

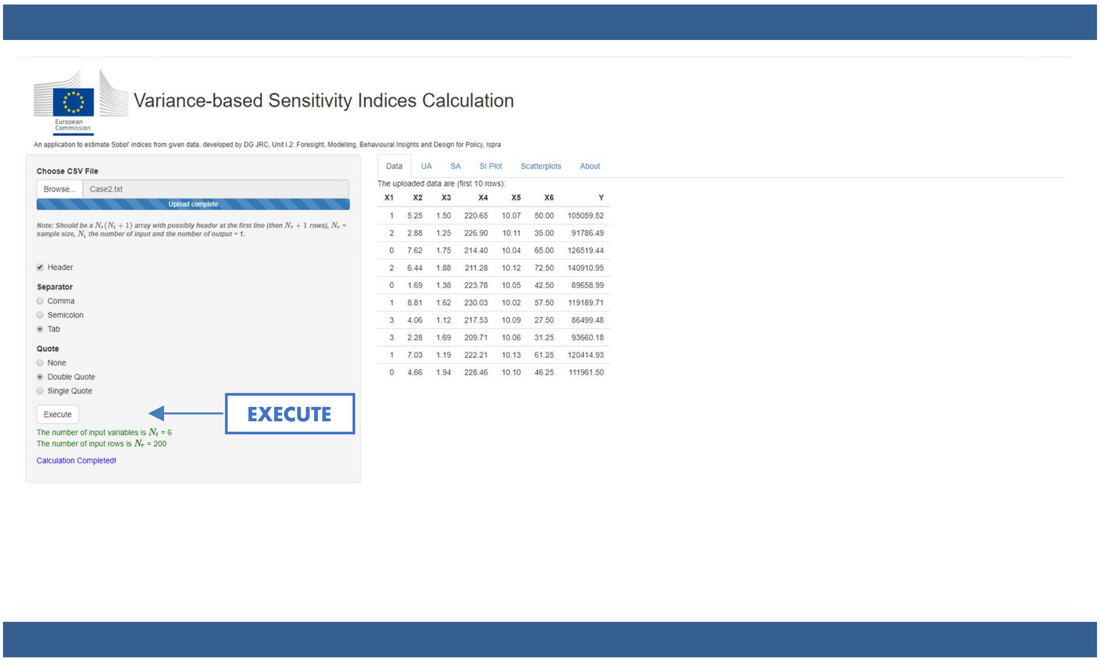
4. Specify the **Separator**. Three kinds of separator are possible between data: comma, semicolon, and tab. An incorrect selection is immediately detected and notified.

5. Specify the kind of **Quote** which has been used for the variable labels. Three different options are available: none, double quote, and single quote.



6. Once the previous steps are completed, the selections are automatically checked and data are uploaded successfully. The result is similar to FIGURE A1-2: the first data (ten rows) of the file are shown and the variable names displayed. At the bottom of the selection pane, the number of the uploaded variables and rows is indicated, together with the message 'Data upload successful'. In the case of any mistake, this information is not available and the incorrect options should be rectified to proceed.

FIGURE A1-2
Successful data upload

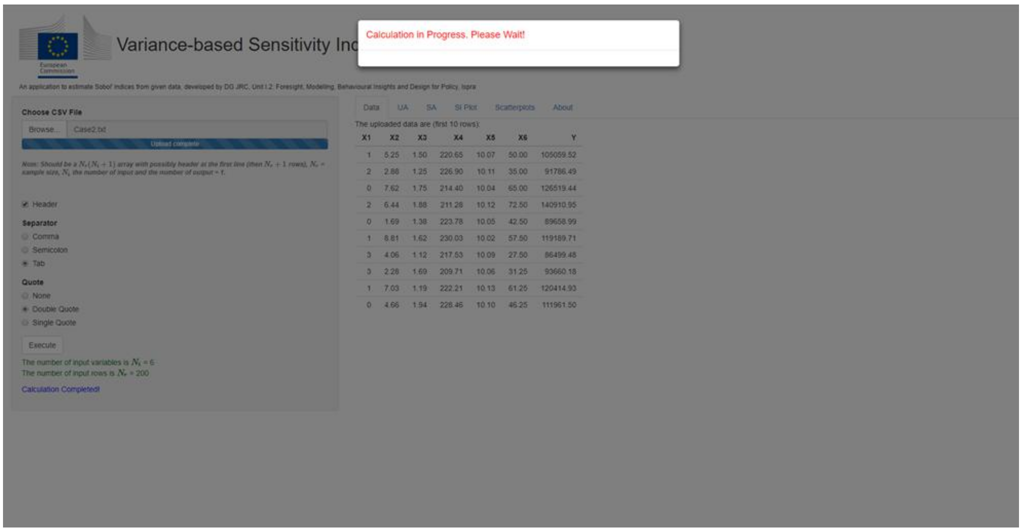


7. If the data upload is successful, it is possible to **Execute** the program.

STEP 2: **Execution of the program**

Clicking the **Execute** button, the UA-SA are launched. During the program execution, the message 'Calculation in Progress. Please Wait' is displayed in red indicating that the computation of the UA-SA is being correctly running (see FIGURE A1-3). Once the calculation is achieved the message 'Calculation Completed!' appears in blue to warn the User.

FIGURE A1-3
Program execution



STEP 3: **Analysis of the UA-SA results**

At this stage, on the right-hand, all the Tabs are active. The UA-SA results are available in the following four Tabs:

- Tab **UA** (FIGURE A1-4): provides some information about the output distribution and its main statistics, such as the mean, median, and 95% confidence interval. The output distribution is shown using a histogram graph and the estimated density function curve is added.

- Tab **SA** (FIGURE A1-5): provides the estimated Sobol' first-order and total-order indices of each variable. The interactions between inputs are also highlighted in a specific section. In addition, some information about the results of the polynomial chaos expansion (PCE) are available, such as N_{pce} = 'Number of terms in the expansion' and Q_{ε}^2= 'amount of variance unexplained' by the PCE approximation.

- Tab **SI Plot** (FIGURE A1-6): the first-order (in red) and total-order indices (in blue) are displayed graphically allowing a faster inference. Both a stacked bars chart and a plot of the indices are available.

- Tab **Main Effects** (FIGURE A1-7): displays the marginal effect of each variable (univariate effect) versus the scatterplots. The marginal effect normally shows the trend of the effect of each variable onto the model response y.

Results (including microdata for scatterplots) can be downloaded in csv format. All pictures and tables can be selected and exported through both the command save or copy.

FIGURE A1-4
Tab UA

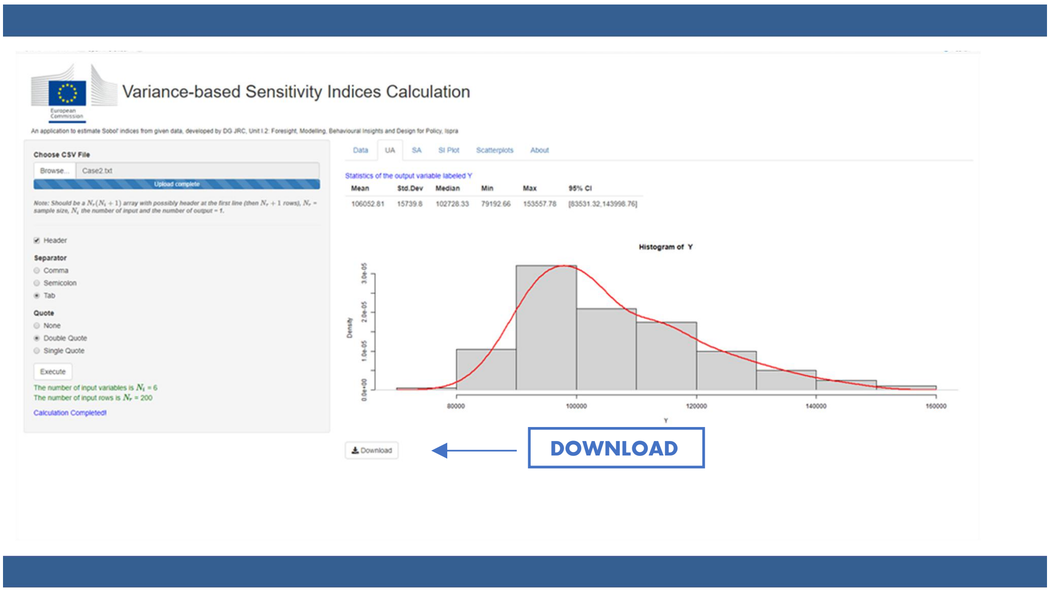


FIGURE A1-4. *Results displayed in the tab UA. Main statistics about the model output are provided. The output distribution is shown in a histogram graph and the estimated density function curve is added in red.*

FIGURE A1-5
Tab SA

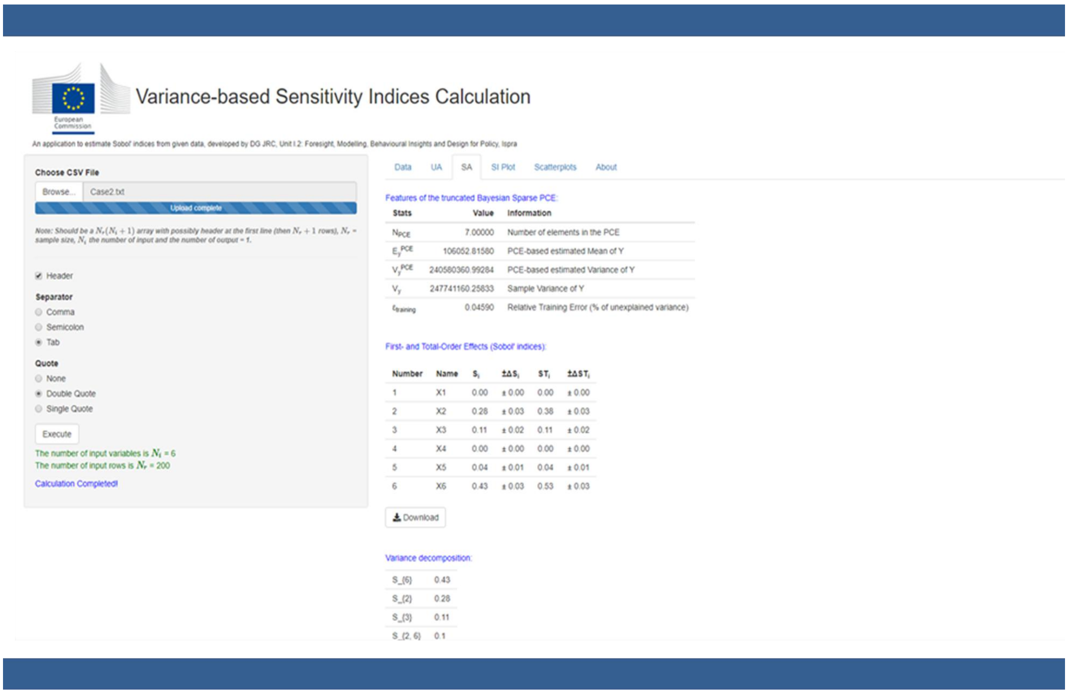


FIGURE A1-5. *Results displayed in the tab SA. In the first table, the results about the estimation procedure are indicated i.e. the number of terms of the PCE and the unexplained variance rate. The estimated first-order sensitivity index and total-order sensitivity index for each variables are shown in the second table. Finally, the variance decomposition is given.*

Figure A1-6
Tab SI Plot

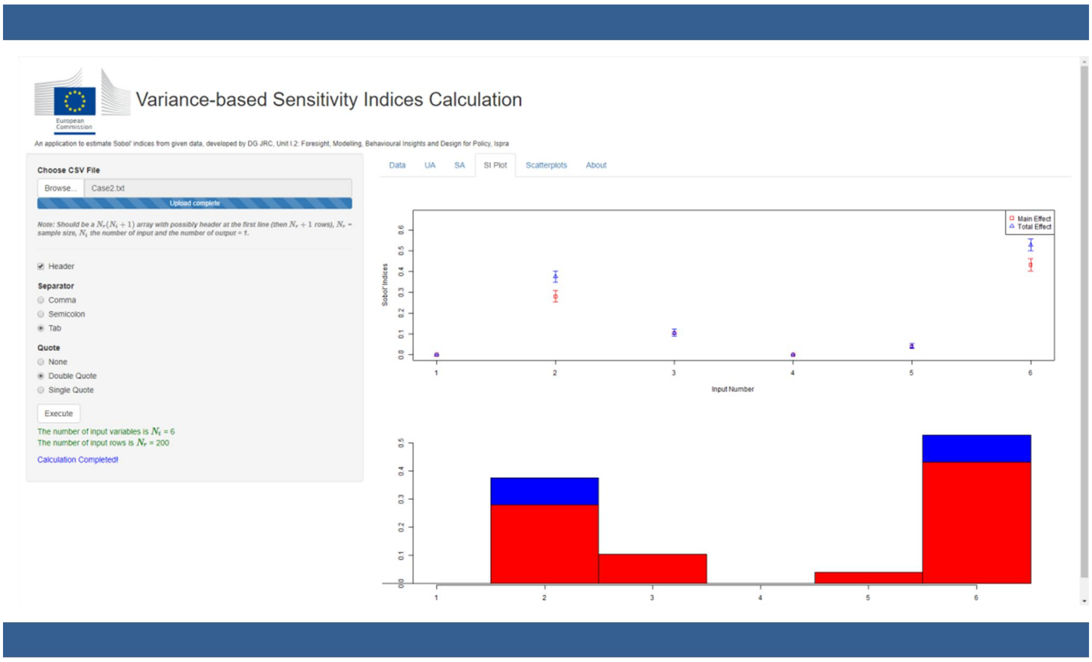


Figure A1-6. *Results displayed in the tab SI Plot. First-order and total-order indices are provided in graphic format.*

Figure A1-7
Tab Main effects

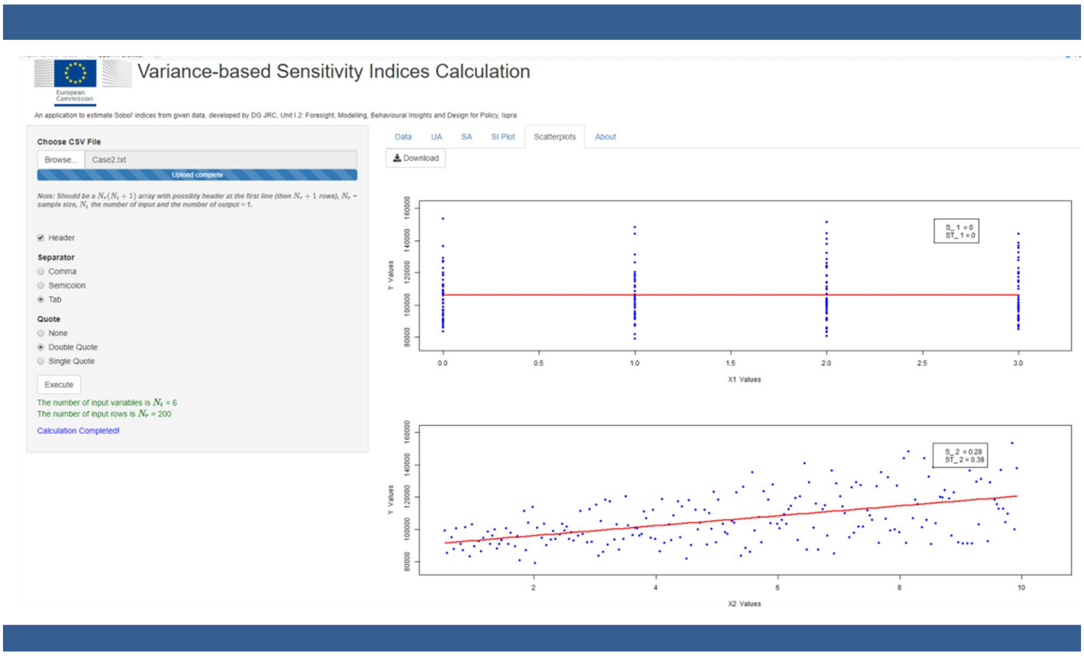


Figure A1-7: *Results displayed in the tab Main Effects. Input and output are plotted in a graph and the linear regression curve is added in red. In a box, the estimated first-order and total-order indices are given.*

Main references:

Homma, T. and Saltelli, A., 1996. Importance measures in global sensitivity analysis of nonlinear models. Reliability Engineering & System Safety, 52(1), pp. 1-17.

Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M, & Tarantola, S., 2008. Global sensitivity analysis: the primer. Probability and Statistics. John Wiley & Sons, Chichester NY.

Shao, Q., Younes, A., Fahs, A., & Mara, T.A., 2017. Bayesian sparse polynomial chaos expansion for global sensitivity analysis, *Computer Methods in Applied Mechanics and Engineering*, 318, pp. 474-496.

Sobol, I.M., 1993. Sensitivity estimates for nonlinear mathematical models. *Mathematical Modelling and Computational Experiments*, 1(4), pp. 407-414.

The SAMO group of the Competence Centre on Modelling provides advice and support on UA-SA. Guidance and software tools are available on our webpage.

Contacts:

EC-CCMOD@ec.europa.eu https://ec.europa.eu/knowledge4policy/modelling/topic/sensitivity-analysis-models_en

Annex 2. Some quantitative insights

Sobol' sensitivity index

In the early nineties, the Russian mathematician I.M. Sobol' (Sobol', 1993) showed how the variance of the model output can be decomposed into summands of increasing dimensionality, laying the foundations of the variance-based sensitivity analysis.

Given a set of independent inputs $\boldsymbol{x}$=(x_1,...,x_d) defined over the input space Ω^d and a square-integrable function y=f($\boldsymbol{x}$) (which can be seen as a scalar model response), the total variance of the latter can be split into the sum of different partial variances (the so-called ANOVA decomposition):

$$\mathrm{V(Y)}=\sum_{i=1}^{\mathrm{d}} \mathrm{V}_i + \sum_{\mathrm{j>i}}^{\mathrm{d}} \mathrm{V}_{i,\mathrm{j}} + \cdots + \mathrm{V}_{1,\ldots,\mathrm{d}}$$

where the summand V_i represents the partial contribution of the input x_i solely (i.e. first-order effect):

$$\mathrm{V}_i = \mathrm{V}(\mathrm{E}(\mathrm{y}|\mathrm{x}_i))$$

while $V_{i,j}$ is the partial variance due to the interaction effect of the pair inputs (x_i, x_j) (second-order effect):

$$\mathrm{V}_{i,\mathrm{j}} = \mathrm{V}_{i,\mathrm{j}}(E(\mathrm{y}|\mathrm{x}_i,\mathrm{x}_\mathrm{j})) - \mathrm{V}_i(\mathrm{E}(\mathrm{y}|\mathrm{x}_i)) - \mathrm{V}_\mathrm{j}(E(\mathrm{y}|\mathrm{x}_\mathrm{j}))$$

and so forth…

By dividing the first equation by the total variance $V(y)$ one yields the so called variance-based sensitivity indices (or Sobol' indices):

$$1 = \sum_{i=1}^{\mathrm{d}} \mathrm{S}_i + \sum_{\mathrm{j>i}}^{\mathrm{d}} \mathrm{S}_{i,j} + \cdots + \mathrm{S}_{1,\ldots,\mathrm{d}}$$

Therefore, the sensitivity indices are normalized values between 0 and 1. They represent the amount of the output variance due to the different possible effects of the model inputs. For instance, the main effect of model input x_i, that is the conditional variance, is measured by $V(E(y|x_i)$. If we divide it by the total variance $V(y)$ of the model output we obtain the first-order Sobol' sensitivity index S_i, also called main effect index of the model input x_i:

$$\mathrm{S}_i = \frac{\mathrm{V(E(y|x}_i))}{\mathrm{V(y)}}$$

A high value of S_i denotes a prominent role of the x_i on the uncertainty in the model output Y, while a low value indicates a negligible influence of the input alone on the outcome uncertainty.

In a similar way, higher sensitivity indices are defined considering higher interactions among inputs and their normalised effects.

The total contribution of x_i to the model uncertainty is expressed by the total-order sensitivity index (Homma & Saltelli, 1996) which considers all the effects of any order involving x_i. The total-order index is defined as follows:

$$\mathrm{ST}_i = 1 - \frac{\mathrm{V(E(y|}\mathbf{x}_{\sim i}))}{\mathrm{V(y)}}$$

where the subscript ~*i* means all inputs except for the *i*-th one.

Thus, given that the total variance can be decomposed as:

$$\mathrm{V(y) = E(V(y|x}_i)) + \mathrm{V(E(y|x}_i))$$

the total-order sensitivity index of x_i can also be defined by:

$$\mathrm{ST}_i = \frac{\mathrm{E(V(y|}\mathbf{x}_{\sim i}))}{\mathrm{V(y)}}$$

The ANOVA decomposition is always possible and unique provided that the model inputs are independent of each other and that the output variance over the input space is a finite number. Therefore, this decomposition is independent of the nature of the input-output relationship. This means that variance-based sensitivity indices are model-free. However, in practice, it can be an issue to estimate numerically the variance of a random variable when the probability distribution of the latter has long-tailed (Borgonovo et al. 2014).

Polynomial chaos expansion (PCE)

Let $y = f(x)$ be the model response of interest. The vector $\boldsymbol{x}$ = ($x_1,\ldots,x_d$) gathers the model inputs which are assumed to be randomly and independently distributed. Polynomial chaos expansion (PCE) is a spectral representation of the input-output mapping, namely,

$$f(\boldsymbol{x}) = \sum_{r_1=0}^{+\infty} \ldots \sum_{r_d=0}^{+\infty} a_{r_1,\ldots,r_d} \psi_{r_1}(x_1)\ldots\psi_{r_d}(x_d)$$

where the $a_{r_1,\ldots,r_d}$'s are the PCE coefficients and the $\psi_{r_i}(x_i)$'s are orthonormal polynomials of degree r_i. Such a representation is very convenient because it allows to inferring that the total variance of $f(\boldsymbol{x})$ can be decomposed as follows:

$$Var[f(\boldsymbol{x})] = \sum_{r_1=0}^{+\infty} \ldots \sum_{r_d=0}^{+\infty} a^2_{r_1,\ldots,r_d}$$

Consequently, it is straightforward to infer that the total contribution of x_i to the total output variance is:

$$VT_i = \sum_{r_1=0}^{+\infty} \ldots \sum_{r_i=1}^{+\infty} \ldots \sum_{r_d=0}^{+\infty} a^2_{r_1,\ldots,r_i,\ldots,r_d}$$

whereas its sole contribution is:

$$V_i = \sum_{r_i=1}^{+\infty} a^2_{0,\ldots,r_i,\ldots,0}$$

Similarly, any partial variance that involves one or more input variables can be inferred. Therefore, the overall Sobol' indices can be obtained, so that:

$$\sum_{s=1}^{d} \sum_{i_t>\ldots>i_s}^{d} S_{i_s,\ldots,i_t} = 1$$

Consequently, the key point with PCE is to estimate the coefficients $a_{r_1,\ldots,r_d}$'s knowing the set of orthonormal polynomial $\psi_{r_i}(x_i)$'s. This can be achieved with the stepwise regression approach of Shao et al. (2017) – see box A2-1. The latter merely requires a Monte Carlo sample of ($\boldsymbol{x}$,y) obtained after drawing N trials of $\boldsymbol{x}$ from its joint probability distribution (recall that $\boldsymbol{x}$ is a random vector) and then, for each trial, running the model and collecting the response of interest y.

Box A2-1. Bayesian SPCE ALGORITHM

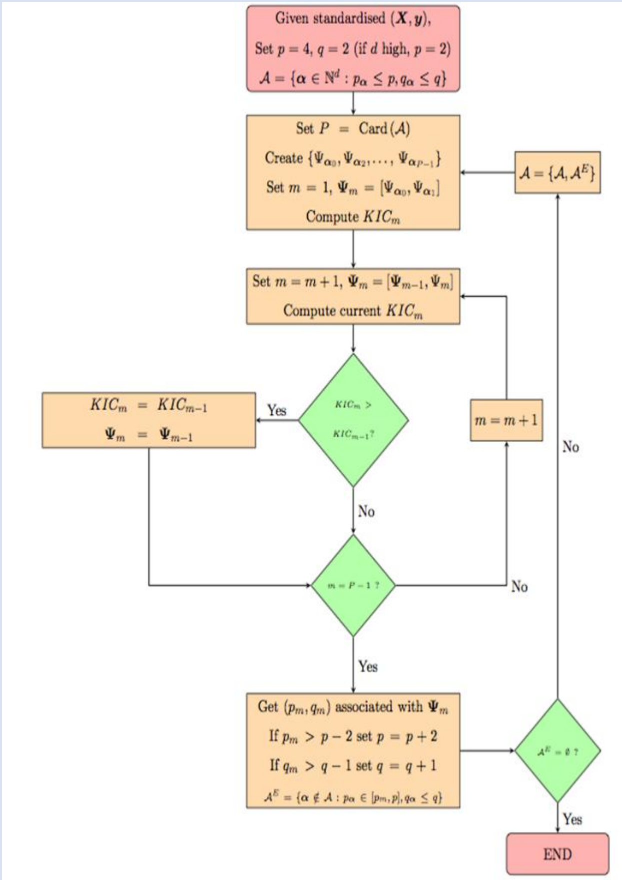
Objective: Find the best subset A and the associated PCE coefficients $\mathbf{a}_\alpha$ from given dataset [**X**,**y**]
Means: Model selection criterion to find A and bayesian inference with informative prior on $\mathbf{a}_\alpha$
Our Choice: Kashyap information criterion and Gaussian prior (i.e. ridge regression)

Likelihood: $L = N(0, \sigma_e^2)$

Prior: $p(\mathbf{a}_\alpha) = N(0, \mathbf{C}_{\mathbf{aa}})$

Coefficients: $\mathbf{a}_\alpha = \sigma_e^{-2}\left(\sigma_e^{-2}\Psi_{\mathbf{m}}^{\mathbf{t}}\Psi_{\mathbf{m}} + \mathbf{C}_{\mathbf{aa}}^{-1}\right)^{-1}\Psi_{\mathbf{m}}^{\mathbf{t}}\mathbf{y}$

KIC: $KIC_m = N\ln\left(\sigma_e^{-2}\right) + \ln\left(\left|\sigma_e^{-2}\Psi_{\mathbf{m}}^{\mathbf{t}}\Psi_{\mathbf{m}} + \mathbf{C}_{\mathbf{aa}}^{-1}\right|\right) + \mathbf{a}_\alpha^{t}\mathbf{C}_{\mathbf{aa}}^{-}$



Annex 3. Sensitivity analysis methodologies – overview

Introduction

In this annex, we provide an overview of the main sensitivity analysis methodologies currently in use. Conceptually, a model ***M*** (Figure A3.1) expresses the relationship between two sets of data (input/output): it provides some output responses given a set of input values $\boldsymbol{x}=(x_1,\ldots,x_d)$. For the sake of convenience, we here assume that there is only one scalar model response of interest y.
From a mathematical point of view, the input/output relationship can be described by the following mapping:

$$y = f(x_1,\ldots,x_d)$$

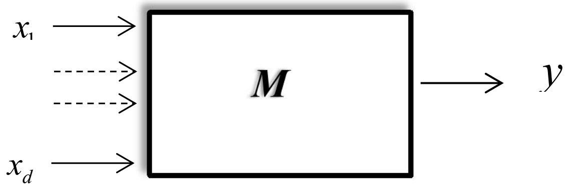


Figure A3.1. Model representation.

In the remainder of the Annex, we explain the different strategies currently in use to perform the sensitivity analysis of a model response.

Methodologies

a) **GSA from given data**

In some situations, the model input/output cannot be chosen by the SA analyst and the only available information is a set of input values with the relative model output, which are therefore qualified as 'given data'.
In this section, we analyse how to infer the importance of the input variables for the response of interest from a given input/output Monte Carlo sample [**X**,**y**]; where **X** is an Nxd matrix and **y** the associated vector of model responses. The i-*th* column of **X** contains the N Monte Carlo draws of x_i.
The Monte Carlo input sample **X** is assumed to have been **independently** drawn. The independence assumption is primordial to facilitate the interpretation of the analysis although not mandatory.

Qualitative GSA with scatterplots

A first simple way to judge whether an input variable x_i has a possible impact on y is to analyse the (x_i,y) scatterplots. Two sets of associated data **X** and **y** can be plotted in the plan, where points show the relationship between them. Referring to a model, it is possible to plot each input (horizontal axes) versus the output (vertical axes) in the plan and the scatterplot is used to investigate whether there is a dependence or not between the displayed I/O.
For example, when the plotting shows the same trend between input and output we detect a positive relationship, on the contrary, when input and output move in different directions

the correlation is negative. Figure A3.2 displays three different scatterplots that lead to the following inferences: i) the plot on the left that x_1 has some influence on y because the input/output relationship is heteroscedastic, that is, the variation of y depends on the value of x_1 (i.e. $V(y|x_1) \neq$ constant), ii) the central plot shows that x_2 is an influential variable for y because one can clearly see a trend in the input/output relationship (it indicates that $E(y|x_2) \neq$ constant), heteroscedasticity is also very clear, and iii) the plot on the right indicates that x_3 is not important for y. This analysis is however only qualitative because one cannot conclude whether x_1 is more important than x_2.

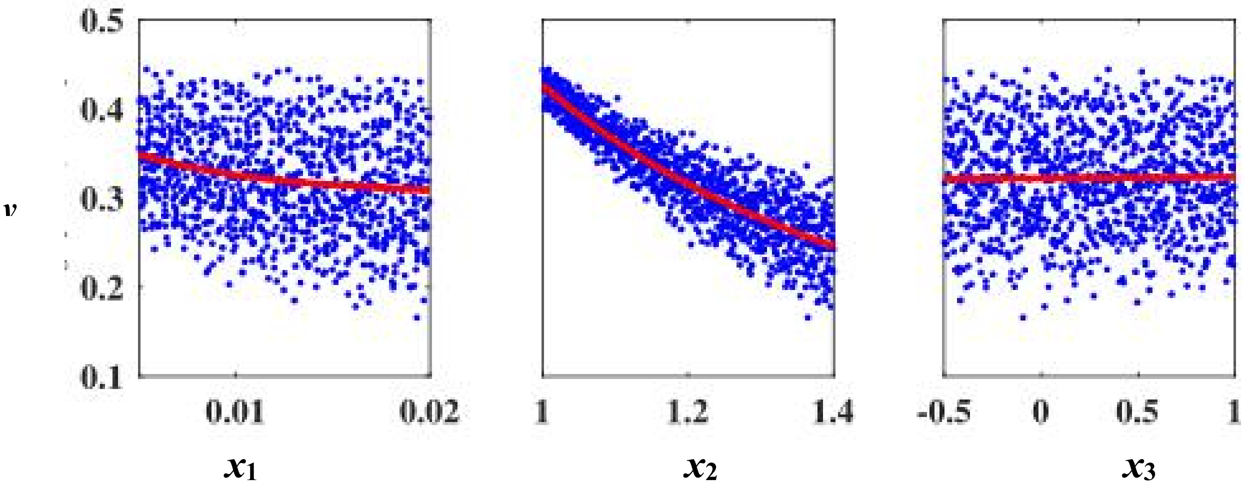


Figure A3.2. Three different scatterplots of y versus some input variable x_i.

Quantitative GSA with regression

An emulator is a simpler model able to approximate (emulate) the original input/output relationship $y = f(x_1,\ldots,x_d)$, that is computationally cheaper to run than the original model $\boldsymbol{M}$. Therefore, emulators (or metamodeling) can be used instead of the original model in an efficient way to compute the sensitivity indices of interest. Most of the emulators are based on regression techniques.

Linear regression: The importance of the input variables can be assessed by fitting a linear function onto the data set. Let us consider the following formula:

$$\bar{y} = \beta_0 + \beta_1\bar{x}_1 + \beta_2\bar{x}_2 + \ldots + \beta_d\bar{x}_d + e$$

where the bar-variables are standardized (i.e. mean 0 and variance 1), and e is an error term[7]. The importance of the variables is measured by $|\beta_i|^2$. The higher the regression coefficient, the more important is the associated variable. The corresponding regression line can be traced in the plan given a visual instrument of analysis (Figure A3.3).

[7] Among the most widely applied 'errors', we can mention the *Mean Absolute Error, Mean Square Error, Mean Absolute Percentage Error,* and *Mean Percentage Error.*

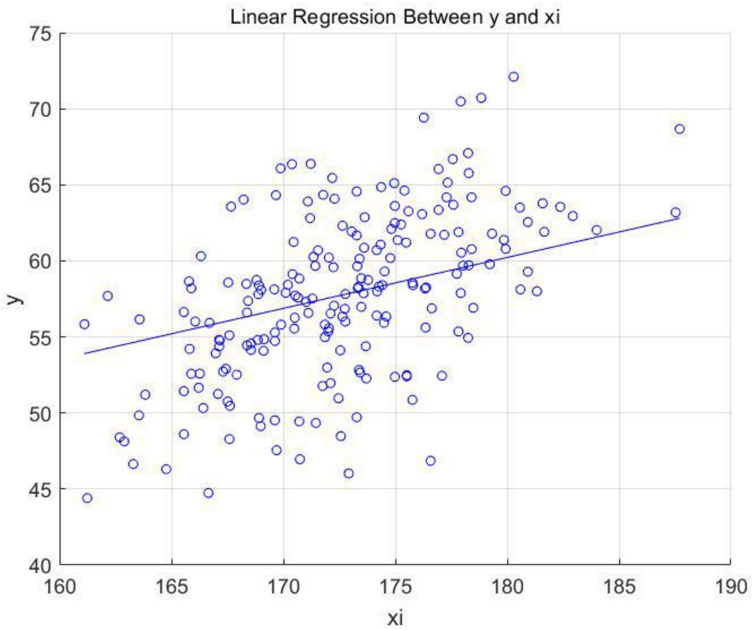


Figure A3.3. I/O plot and linear regression.

Linear regression is a very useful (and simple) method in SA but the provided information is insufficient with non-linear/non-additive models. The GSA is judged successful if the variance of the error V(e) ~ 0, otherwise one has to consider non-linear regression.

Additive regression: A non-linear additive regression relies on the fitting of the data set onto a multivariate function of the form:

$$y = f_0 + f_1(x_1) + f_2(x_2) + \dots + f_d(x_d) + e$$

often the non-linear functions are chosen as a polynomial of degree p: $f_i(x_i) = \sum_{k=1}^{p} x_i^k \dots$ but other choices are possible. The importance of the variables is inferred by computing and comparing the first-order sensitivity index:

$$\hat{S}_i = \frac{V(f_i(x_i))}{V(y)}$$

The higher the first-order sensitivity index, the more the associated variable is important. The GSA is judged successful if the variance V(e) ~ 0, otherwise one has to consider non-additive regression.

Non-additive regression: The utmost non-linear regression method that can be applied stems from the ANOVA decomposition which has the following form (Sobol' 1993):

$$y = f_0 + \sum_{i_1=1}^{d} f_{i_1}(x_{i_1}) + \sum_{i_2 > i_1}^{d} f_{i_1,i_2}(x_{i_1}, x_{i_2}) + \dots + f_{i_1,\dots,i_d}(x_1, \dots, x_d) + e$$

where for convenience the **functions** in the decomposition are chosen **orthogonal**. The importance of the variables by computing and comparing the first-order sensitivity index and the total-order sensitivity index is given by:

$$\widehat{ST}_i = \frac{\sum_{\boldsymbol{u}_i} V\left(f_{\boldsymbol{u}_i}(\boldsymbol{x}_{\boldsymbol{u}_i})\right)}{V(y)}$$

the subset $\boldsymbol{x}_{\boldsymbol{u}_i}$ is any subset of $\boldsymbol{x}$ that contains the variable x_i (i.e. $\boldsymbol{x}_{\boldsymbol{u}_i} \subseteq \boldsymbol{x}{:}x_i \in \boldsymbol{x}_{\boldsymbol{u}_i}$). We note that the total-order index $\widehat{ST}_i \geq \hat{S}_i$ and contains all the relative contribution of x_i to the variance of y. An input is deemed non-important if its total-order sensitivity index is zero.

The Bayesian sparse polynomial chaos expansion of Shao et al. (2017) implements such a non-linear regression. This method is implemented in the WebApp developed for EC staff and available at https://web.jrc.ec.europa.eu/rapps/sensitivity/ (see section 5 and Annex 1).

Quantitative GSA with partitioning

Another way to assess the importance of the input variable x_i is to measure how the probability density function (pdf) conditioned onto x_i, namely $p(y|x_i)$, differs from the unconditional pdf $p(y)$. Instead, one can also compare the cumulative density function (cdf, denoted respectively $F(y|x_i)$ and $F(y)$). From given data, to estimate the condition densities one cannot fix the value of x_i, but the input range can be split, for example, into n non-overlapping intervals I_k, k=1,…,n, and then the conditional pdf (or cdf) can be estimated: $\hat{p}(y|x_i \in I_k)$. This is illustrated in Figure A3.4.

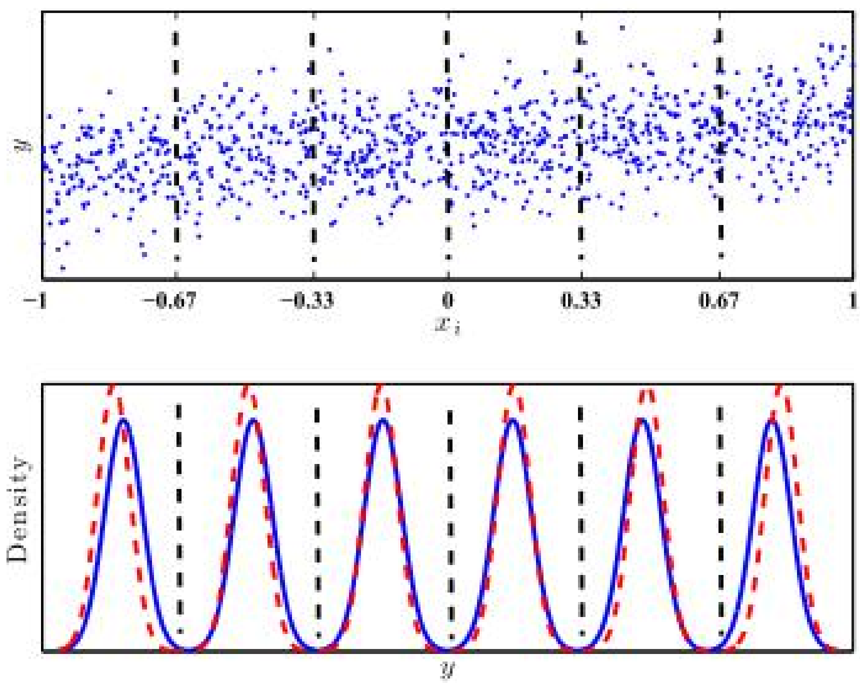


Figure A3.4. Top - scatterplots of y versus input variable x_i with the range of the latter split into intervals. Bottom – the pdf of the sub-samples within each interval (conditional pdf) is compared with the pdf of the entire sample (unconditional pdf).

pdf-based sensitivity index (Plischke et al., 2013): The statistic to be computed in order to obtain a sensitivity index is the following:

$$\widehat{d}_i^{(k)} = \int_{\Re} |\hat{p}(y) - \hat{p}(y|x_i \in I_k)|\, dy$$

and the sensitivity measure of interest is:

$$\hat{\delta}_i = \frac{1}{N}\sum_{k=1}^{n} N_k\, \widehat{d}_i^{(k)}$$

where N_k is the number of draws in the sub-range I_k.

cdf-based sensitivity index (Pianosi et al., 2015): The statistic to be computed in order to obtain a sensitivity index is the following:

$$\hat{t}_i^{(k)} = \max_y |\widehat{F}(y) - \widehat{F}(y|x_i \in I_k)|$$

and the sensitivity measure of interest is:

$$\hat{\tau}_i = \frac{1}{N}\sum_{k=1}^{n} N_k\, \hat{t}_i^{(k)}$$

Monte Carlo filtering (Hornberger et al., 1981):
Monte Carlo filtering (MCF) is used when we are not interested in the precise values of the output Y of a model, and we can split them into two distinct classes such as "*acceptable*" or "*not-acceptable*", "*permitted*" or "*not-permitted*", "*0*" or "*1*" (see also Figure A3.5). This idea of defining as "*permitted"* or "*not-permitted*" the model action is particularly suitable for scenarios where the output is subject to certain constraints, such as staying between certain bounds or below a given threshold. Therefore, MCF can be seen as a special case of the partitioning approaches previously discussed in which only two partitions are considered (n = 2): the one containing acceptable draws and the other containing non-acceptable draws.
Monte Carlo filtering can only capture effects on the model related with single input factors and cannot detect interactions among factors.

The estimation of these probability distributions can be done in different ways, for example in Hornberger et al. (1981) and Saltelli et al. (2004) two different version of Kolmogorov-Smirnov test are used.

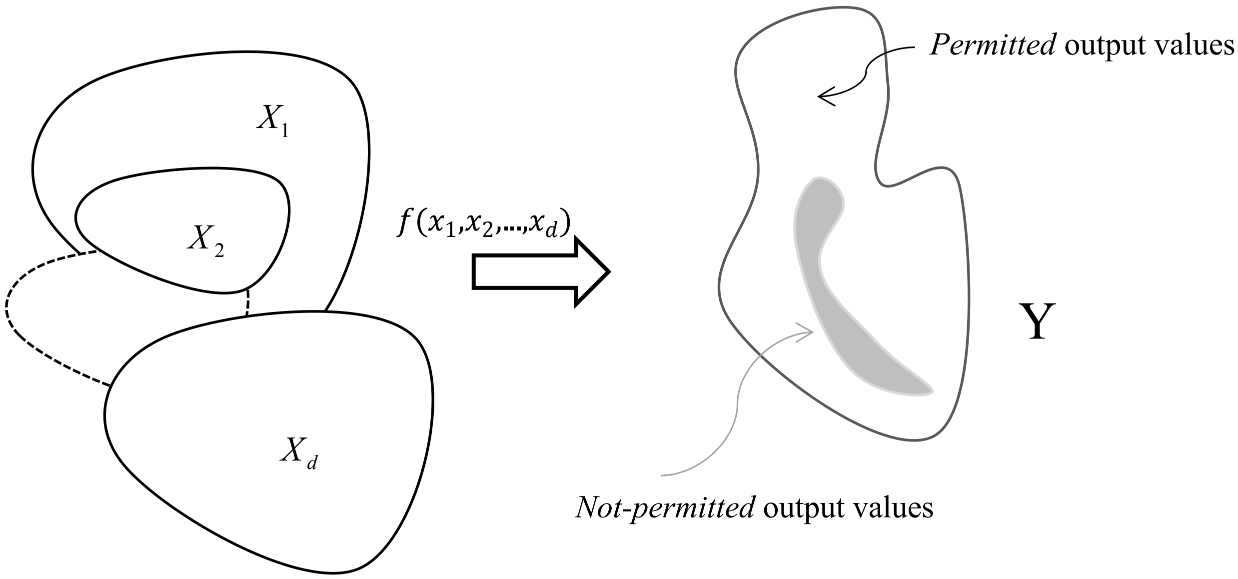


Figure A3.5. Model output categorization into two classes.

b) GSA from specific design

The advantages of the previous approaches are that they only require one Monte Carlo sample of size N. But depending on the method used their results may be inaccurate or they can possibly fail. Besides, most of them do not allow us to cope with groups of input variables. There are other approaches proposed in the literature that overcome some of these issues. They are usually more computationally demanding. They are briefly described hereafter.

Screening method (Morris, 1991): Screening methods have their roots in a field of Applied Statistics called *design of experiments.* Design of experiments is formally defined as: *a systematic method to determine the relationship between factors affecting a process and the output of that process*.
In very simple terms, if we consider a recipe as a 'system' to cook food, for example a muffin, the final result (the muffins) will depend on various factors: the amount of flour, the number of eggs, the oven temperature etc…Each of these factors has an impact on the final outcome. A well-planned and executed set of experiments on how to obtain a good muffin may provide us with the valuable information regarding the best option in terms the ingredients and muffins.
Among the main screening methods, the Morris OAT design (1991) allows us to detect the non-important input variables by computing the elementary effects of the inputs at different points in the input space. The sampling strategy is based on the One-At-a-Time (OAT) approach for a total cost of N=(rd + 1) runs (or $r(d$ + 1) when using radial sampling). The elementary effect is defined as follows:

$$EE_i^{(k)} = \frac{f\big(x_{1,r},x_{2,r},\ldots,(x_{i,r}+\Delta_k),x_{i+1,r},\ldots,x_{d,r}\big) - f(\boldsymbol{x_r})}{\Delta_k}$$

The sensitivity index of interest with the Morris method is:

$$\mu_i^* = \frac{1}{r}\sum_{k=1}^{r}\left|EE_i^{(k)}\right|$$

The Morris method is qualitative in the sense that one cannot rely on μ_i^* to rank the inputs by order of importance.

Monte Carlo estimators of variance-based sensitivity indices (Sobol', 1993): As thoroughly discussed in this report, first-order and total-order variance-based sensitivity indices can be estimated with Monte Carlo estimates of integral. They can deal with groups of inputs. The best estimators (more accurate) require $N=2N_k(d+1)$ model runs.

FAST (Saltelli et al., 1999): The Fourier Amplitude Sensitivity Test (FAST) also allows for estimating the overall first-order and total-order variance-based sensitivity indices. FAST reaches this goal by generating periodic samples of each input variable x_i and then using a Fourier analysis to decompose the variance of the model output y. It requires $N=N_k \times d$ model runs. Nowadays, FAST methods are not so popular in particular as the choice of the frequency set to sample the input variables is a delicate problem.

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