Interval-Based Global Sensitivity Analysis for Epistemic Uncertainty

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The objective of sensitivity analysis is to understand how the input uncertainty of a mathematical model contributes to its output uncertainty. In the context of a digital twin, sensitivity analysis is paramount for the automatic verification and validation of physical models, and can also be used as a decision support tool to determine on which parameter to invest more empirical effort. Yet, sensitivity analysis often requires making assumptions about the inputs such as probability distribution functions, as it is the case in variance-based methods, or relies on surrogate models that also introduce more assumptions, as in kriging or polynomial chaos. It can be the case that one cannot reliably assign probability distribution functions if the model is dominated by epistemic uncertainties, or the complexity of the model is such that surrogate models cannot accurately capture its behaviour.
We present a non-probabilistic sensitivity analysis method which requires no assumptions about the input probability distributions: the uncertainty in the input is expressed in the form of intervals, and employs the width of the output interval as the only measure, in the same way that interval analysis. As a positive by-product, the method also returns all the information that could be obtained with the reduction of the input interval to a single value, also called pinching. We use the Ishigami function as test case to show the performance of the proposed method, and compare it with Sobol indices.

Keywords: epistemic uncertainty, uncertainty quantification, sensitivity analysis, interval arithmetic, sobol indices, digital twin.

1. Introduction

Prediction is inherent to science since prediction is essential to test theories and their consequences. Thanks to the power of modern computation, the prediction of natural phenomena represented by mathematical models can now be tested at unprecedented scales. Digital twins attempt to exploit this advantage by modelling physical systems and allowing their evaluation via simulation, as these systems are often technically and economically prohibitive to operate in the physical world (Wagg et al. (2020)). However, digital twins are often so complex that it is not possible to infer their prediction from experience and judgement alone. Therefore, it is desirable to verify and validate the prediction of these models without having to rely on subjectivity (Azzini et al. (2020)). Sensitivity analysis can help with this task, by indicating what model parameters are responsible for the prediction of the model, and how that prediction depends on them (Saltelli et al. (2004)).

Generally, sensitivity analysis methods fall within three categories: derivative-based, distribution-based, and regression-based Razavi et al. (2021). Derivative-based approaches attempt to compute the derivative of the model functions,

Proceedings of the 32nd European Safety and Reliability Conference.
Edited by Maria Chiara Leva, Edoardo Patelli, Luca Podofillini and Simon Wilson

ISBN: 981-973-0000-00-0 :: doi: 10.3850/981-973-0000-00-0_esrel2022-paper

either analytically or numerically, and measure the change in the output when the inputs are perturbed around a base point ([reference]). Distribution-based methods, such as Sobol' indices, decompose the output variance and assigns the partitions to the input variances, indicating how much of the output variance is caused by each input variance (Saltelli et al. (2010)). Lastly, regression-based approaches employ correlation coefficients, regression coefficients, or other machine learning methods (Sudret (2008)).

However, these approaches present some limitations that can make them unsuitable in certain cases. For instance, the analytical description of the functions in the model are not always available, since it is not uncommon to deal with black-box models or models with too many functions that make unpractical or difficult their analytical derivation. Also, derivative-based methods require defining a base point for each input parameter, and a perturbation size. It is not rare to find a situation where there is not consensus about those elements. A similar argument can be made for distribution-based methods, which require a precise definition of the probability distribution functions of the model input parameters. Lastly, to successfully apply regression-based methods, it is necessary to know the behavior of the model under investigation, which is not always known. For example, partial correlation coefficients assume model linearity, or monotonicity in the case of partial rank coefficients (Saltelli and Marivoet (1990)). For these reasons, it is desirable to find a sensitivity analysis method that:

- Does not require knowing the analytical description of the model functions.
- Does not require defining base values for any input parameter.
- Does not require to assume that the input parameters follow a precise probability distribution function.
- Does not depend on the model behavior.

This paper attempts to present an interval-based global sensitivity analysis method that fulfills these requirements. Section 2 introduces some basic concepts in interval uncertainty propagation which are required to perform the analysis. In Section 3 it is explained how the sensitivity indices are calculated in the interval approach, and the pinching measure that can be calculated additionally. Lastly, Section 4 compares the performance of the interval-based method against Sobol' indices in two test cases for the Ishigami function, followed by the conclusion in section 5.

2. Interval Analysis

With interval analysis is possible to set bounds to the output of a model function. When capturing the rigorous enclosure of a model output one can know with certainty what the model represents, and decide whether it adequately depicts reality or not. Also, expressing parameter uncertainties in the form of intervals has the advantage of requiring no assumptions about the uncertainty, making intervals suitable to capture epistemic uncertainty.

The two main methods to compute with intervals are interval arithmetic and sampling. In the former, the mathematical operations are replaced to account for intervals as in Moore et al. (2009). This method requires access to the analytical description of the models (i.e. source code) to make them suitable for interval arithmetic. Sampling methods, on the other hand, do not require to adapt the source code for interval arithmetic. A typical sampling procedure begins assuming uniform distributions for the uncertain parameters, performing the sampling using the Latin Hypercube algorithm, and extracting the minimum and maximum of the outputs of interest (i.e. their interval) Helton et al. (2010). The main drawback of sampling methods is that the resulting output interval will be an inner approximation instead of an outer approximation (when quantifying uncertainty it is better to be safe than sorry).

The sensitivity analysis presented in this paper can be applied with both methods of interval analysis, employing the widths of the input and output intervals as the only required measures. Therefore, it can be used with black-box or sophisticated models that cannot be adapted to work with interval arithmetic (and therefore the uncertainty propagation has to be performed via sampling), or with models which already adopt interval arithmetic.

3. Interval-Based Sensitivity Index

The proposed sensitivity index captures the dependence of the model output on the inputs measuring the area described by these. Figure 1 serves as an illustrative example. It shows the scatterplots of the evaluation of a black-box function $y = f(x_1, x_2)$ with $x_1, x_2 \in [-5, 5]$, with samples generated using Latin Hypercube sampling. As explained in Helton and Davis (2003), scatterplot visualization is a straightforward qualitative method of inspecting dependencies in a model. In this example it is possible to see how y has a linear dependence with x_1 (Figure 1 (a)), but shows little or no dependence with x_2 (Figure 2 (b)). The objective is to turn this qualitative *intuition* into a measurement.

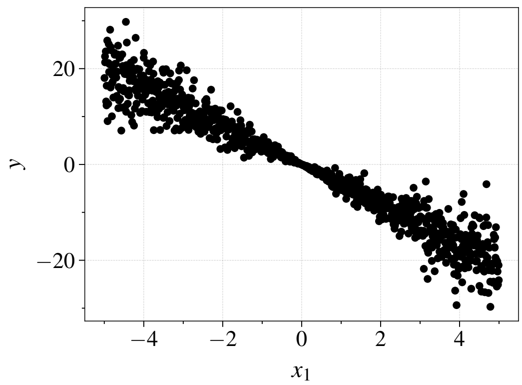
The dependence can be captured measuring the area described by the scatterplot, and comparing it to the box defined by $(\underline{y}, \overline{y}) \times (\underline{x_i}, \overline{x_i})$, where $\underline{y}, \overline{y}$ are the measured minimum and maximum of y, and $\underline{x_i}, \overline{x_i}$ the minimum and maximum of the $i - th$ input parameter. If the measured area equals to the box area, then it can be said that the output has no dependence on that input. If the measured area has a value of 0, it means that the output is determined by that input. Then, any other degree of dependence will fall in-between these two extreme cases. It is important to note that the measurement of the output area will be an approximation of the actual area, being a consequence of the sampling method or the subintervalization if interval arithmetic is employed to solve the model functions. The approximation can be improved increasing the number of samples or subintervals, to the detriment of computational cost.

The sensitivity index is calculated with the following formula

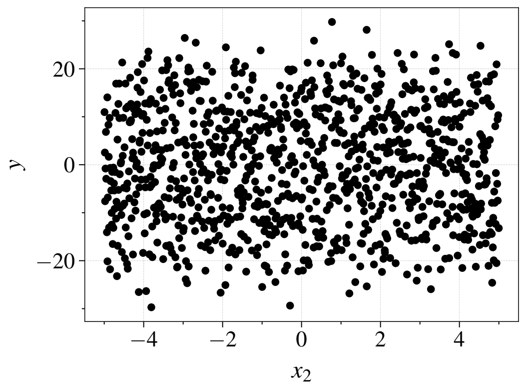
$$S_i = 1 - \frac{\sum_n^N (\underline{x_i}, \overline{x_i})_n \times (\underline{y}, \overline{y})_n}{(\underline{y}, \overline{y}) \times (\underline{x_i}, \overline{x_i})}, \qquad (1)$$

where N is the total number of subintervals. Therefore, S_i is a sensitivity index ranging from 0 (i.e. y is independent of x_i) to 1 (i.e. y is determined by x_i).

The area can be calculated with two different methods depending on whether interval arithmetic was employed to calculate the functions or it was done though sampling. In the case of interval arithmetic the calculation is straightforward as the subintervals can be recycled and the rectangles described by these can be easily computed. On the other hand, if sampling methods were chosen, then the area can be calculated employing an integration method similar to the trapezoidal rule: a step size is defined to sweep through subintervals of x_i in the data, the minimum $\underline{y}$ and maximum $\overline{y}$ are retrieved for each subinterval, and the rectangle area is computed as usual. The main drawback of the integration method is that a step size has to be defined manually, and the impact of this parameter on the proposed sensitivity analysis



(a) Scatterplot of $y = f(x_1, x_2)$ and x_1.



(b) Scatterplot of $y = f(x_1, x_2)$ and x_2.

Fig. 1. Results of the evaluation of a black-box function $y = f(x_1, x_2)$ with $x_1, x_2 \in [-5, -5]$ using 1000 samples generated with Latin Hypercube sampling.

method has not been studied yet. However, since the method is similar to the trapezoidal rule, it may be possible to place error bounds on the accuracy of the sensitivity index.

Figure 2 shows how the areas would be calculated from Figure 1 with the sampling approach. The algorithm requires the output and input data, and the number of subintervals to divide it (20 were used in this example). Then the minimum and maximum output are found for each subinterval, and the area of the rectangle is calculated. The total measured area defined by the scatterplot would be the sum of all the rectangles.

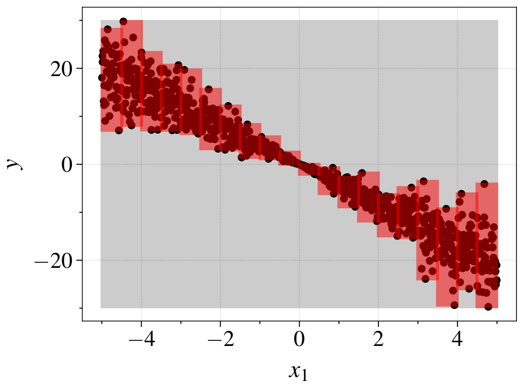
Figure 3 shows the 20 subintervals computed with interval arithmetic using the IntervalArithmetic.jl Julia package (Benet and Sanders (2020)). Note that since the function $y = f(x_1, x_2)$ is a black-box function, the access to its analytical form is restricted, and therefore the interval arithmetic approach would not be possible. However, it has been included as an example to show how the interval arithmetic approach would work.

The sensitivity indices for x_1, x_2 calculated with the sampling and arithmetic approaches are displayed in Table 1. Both approaches return the same ordering, indicating that x_1 is the dominant parameter. Note that the interval arithmetic approach captures that x_2 has no impact on the uncertainty of y (it also can be seen in Figure 3b, since the red area equals to the grey area, making $S_2 = 0$), whilst the sampling approach is not that precise. This is caused by the fact that the sampling approach is an inner approximation method, and the greater the number of samples, the more accurate the sensitivity index is.

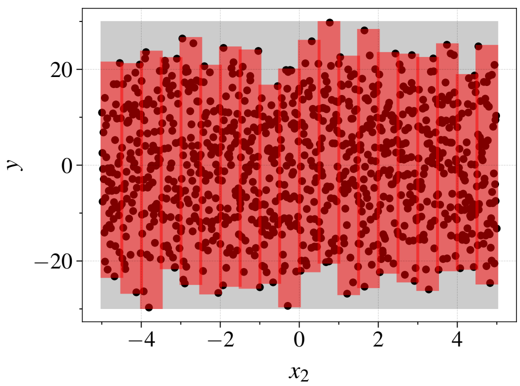
Table 1. Sensitivity indices for x_1 and x_2 with sampling and arithmetic approaches.

Index	Sampling	Interval Arithmetic
S_1	0.790	0.732
S_2	0.197	~ 0

Lastly, an important by-product of the proposed sensitivity index is that its calculation also entails the so called *pinching* method. The *pinching* sensitivity analysis calculates the reduction on the output uncertainty when the uncertainty of an input is reduced from the interval to a single value (e.g., see Ferson and Tucker (2006); Gray et al. (2022)). One drawback of this method is that a single value for each input interval has to be chosen (or several values within the interval, with the consequent increase of computational cost). However, the interval-based sensitivity index retrieves all the *pinching* information possible for



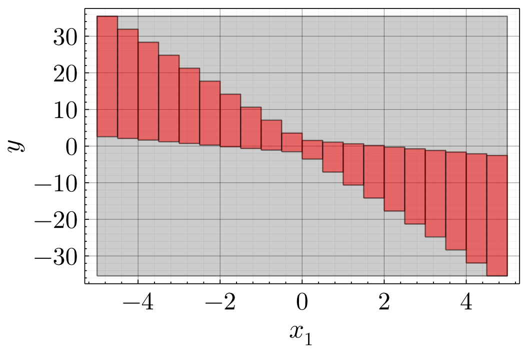
(a) Measured scatterplot area (red) and box area (grey) of $y = f(x_1, x_2)$ and x_1.



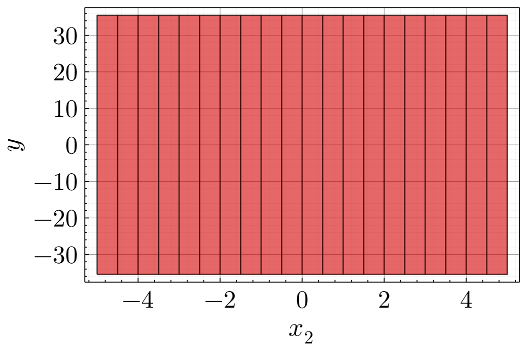
(b) Measured scatterplot area (red) and box area (grey) of $y = f(x_1, x_2)$ and x_2.

Fig. 2. Results of the evaluation of $y = f(x_1, x_2)$ with $x_1, x_2 \in [-5, -5]$ using 1000 samples generated with Latin Hypercube and 20 subintervals. The sensitivity index is calculated as in Eq. (1), where the numerator is equal to the area coloured in red and the denominator equal to the area coloured in grey.

the given number of subintervals; so not only the output dependence on the input is measured, but also how the input affects the output across its domain. Figure 4 shows how reducing uncertainty in x_2 entails no reduction on the uncertainty of y, whilst reducing the uncertainty on x_1 has different consequences on the uncertainty of y depending on the value of x_1. For example, the maximum output uncertainty reduction is obtained pinching at $x_1 = 0$.



(a) Visualisation of the 20 subintervals of $y = f(x_1, x_2)$ and x_1.



(b) Visualisation of the 20 subintervals of $y = f(x_1, x_2)$ and x_2.

Fig. 3. Results of the evaluation of $y = f(x_1, x_2)$ with $x_1, x_2 \in [-5, -5]$ using 20 subintervals and interval arithmetic. The sensitivity index is calculated as in Eq. (1), where the numerator is equal to the area coloured in red and the denominator equal to the area coloured in grey.

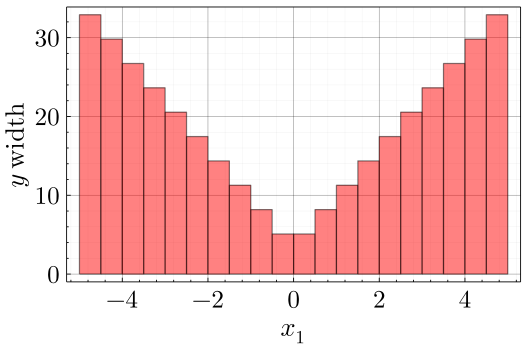
4. Application

To show the performance of the interval-based global sensitivity analysis method proposed, we compare its results in terms of parameter ranking with the Sobol' indices on the Ishigami function, which is common in the uncertainty quantification and sensitivity analysis community for its nonlinearity, nonmonotonicity, and the interaction effects between x_1 and x_3 (Ishigami and Homma (1990)).

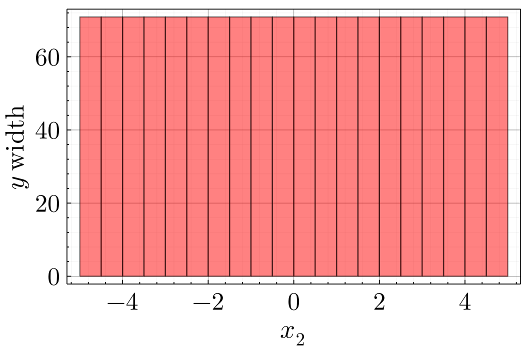
The Ishigami function can be written as

$$f(x_1, x_2, x_3) = \sin(x_1) + a\sin^2(x_2) + b\sin(x_1)x_3^4, \tag{2}$$

where the constants are set to $a = 5$ and $b =$



(a) Output width of y across x_1.



(a) Output width of y across x_2.

Fig. 4. Output width of $y = f(x_1, x_2)$ across the domain of x_1 and x_2. This method calculates the output uncertainty when reducing the input parameter uncertainty to a subinterval or point value.

0.1, and the input variables x_1, x_2, x_3 are independent and uniformly distributed over $[-\pi, \pi]$.

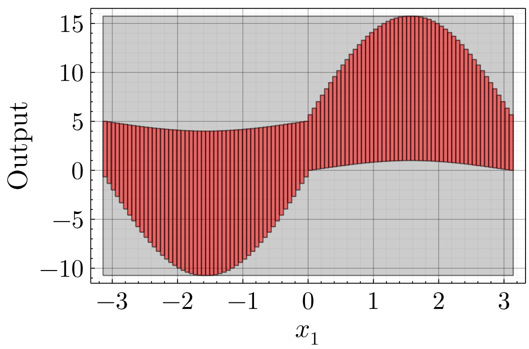
Since the analytical formula of the function is known, the interval-based sensitivity analysis can be performed with interval arithmetic. Figure 5 shows the results of the interval analysis of the Ishigami function with 100 subintervals for x_1, x_2, and x_3, with their corresponding sensitivity indices indicated in Table 2, calculated following the methodology presented in Section 3. According to the interval-based method, the Ishigami function has the highest dependence with x_3, followed by x_1.

Table 2. Interval-based sensitivity indices of the Ishigami function with $x_1, x_2, x_3 \in [-\pi, \pi]$ using interval arithmetic and 100 subintervals.

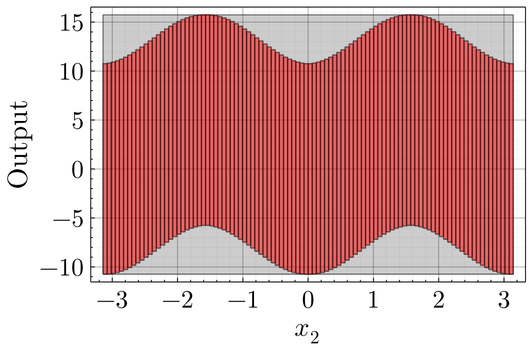
Index	Interval-Based
S_1	0.568
S_2	0.181
S_3	0.581

In addition to the sensitivity indices, the interval-based approach also provides all the information of the *pinching* analysis. Figure 6 shows the uncertainty on the Ishigami output when pinching x_1, x_2, and x_3. The maximum reduction on the Ishigami uncertainty is achieved when x_1 is fixed to $-\pi$, 0, or pi. If pinching any of the three parameters to a point value were not possible, the second best strategy to maximise the output uncertainty reduction would be to pinch the x_3 interval from $[-\pi, \pi]$ to $[-1, 1]$, as Figure 6 (c) suggests. Lastly, pinching x_2 entails almost the same uncertainty reduction, and the smallest of the three parameters, across its entire domain.

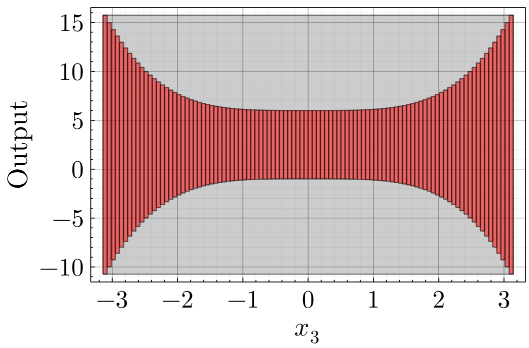
The analytical description for the variance terms used to calculate the Sobol' indices of the Ishigami function are known when the input variables follow an uniform distribution; therefore the *true* total and first order Sobol' indices can be calculated. Table 3 contains the analytical Sobol' indices of the Ishigami function. Analytically, the variance of x_1 is the greatest contributor to the



(a) Intervalisation of the Ishigami function and x_1 using 100 subintervals.



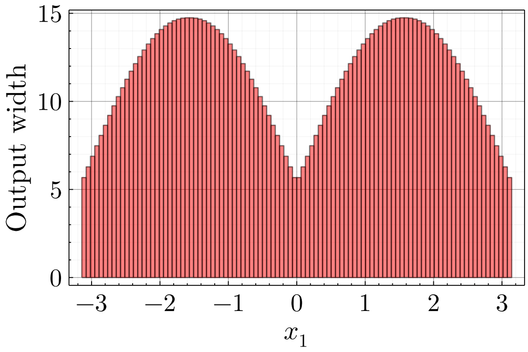
(b) Intervalisation of the Ishigami function and x_2 using 100 subintervals.



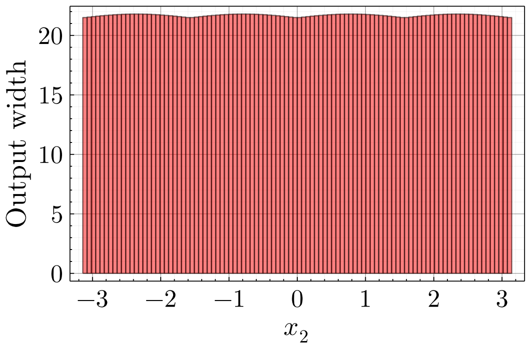
(c) Intervalisation of the Ishigami function and x_3 using 100 subintervals.

Fig. 5. Results of the evaluation of the Ishigami function with $x_1, x_2, x_3 \in [-\pi, \pi]$ with interval arithmetic using 100 subintervals.

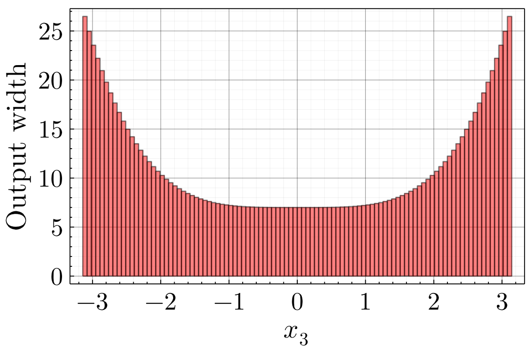
variance of the Ishigami function, and x_3 has effect on the Ishigami only when interacting with x_1.



(a) Output width of the Ishigami function across x_1.



(b) Output width of the Ishigami function across x_2.



(c) Output width of the Ishigami function across x_3.

Fig. 6. Output width of the Ishigami function across the domain of x_1, x_2, and x_3.

Table 3. Analytical first order and total Sobol' indices of the Ishigami function with x_1, x_2, x_3 following an uniform distribution in $[-\pi, \pi]$.

Index	First Order	Total
S_1	0.400	0.711
S_2	0.288	0.288
S_3	0.0	0.311

A second case for the Ishigami function has been included where the input variables follow a triangular distribution in $[-\pi, \pi]$ with mode in 0 instead of an uniform distribution; this case will support the issue when the distribution functions of the input variables are not totally known, showing that the Sobol' indices could be sensible to these assumptions. To calculate the Sobol' indices for the triangular case, 2048 samples were generated using the Saltelli sampling method, which is an extension of the Sobol' sequence optimised for calculating the indices (Saltelli (2002)). Table 4 shows the results of the analysis. The results suggest that, in this case, the variance of x_2 is the greatest contributor to the variance of the Ishigami. Note that the uncertainties on the indices have been omitted since these were negligible, and had no impact on the final parameter ranking.

Table 4. First order and total Sobol' indices of the Ishigami function with x_1, x_2, x_3 following a triangular distribution in $[-\pi, \pi]$ with mode in 0.

Index	First Order	Total
S_1	0.254	0.409
S_2	0.591	0.591
S_3	~ 0	0.158

5. Discussion

6. Conclusion

This paper introduces an interval-based method for performing global sensitivity analysis with interval analysis, performed either via sampling or with interval arithmetic. This method only requires expressing the input parameter uncertainty in the form of intervals, and therefore is particularly suited for cases under epistemic uncertainty. Also, calculating the interval-based sensitivity indices also provides A comparison with the Sobol' indices on the Ishigami function Sobol' indices can return contradictory results

Acknowledgement

This research was funded by the EPSRC and ESRC CDT in Risk and Uncertainty (EP/L015927/1), established within the Institute for Risk and Uncertainty at the University of Liverpool. This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

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