

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 of paramount importance for the automatic verification and validation of physical models, and the identification of parameters which require more empirical investment. Yet, sensitivity analysis often requires making assumptions, e.g., about the probability distribution functions of the input factors, about the model itself, or relies on surrogate models for the evaluation of the sensitivity that also introduce more assumptions. 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. We use the Ishigami function as test case to show the performance of the proposed method, and compare it with Sobol' indices.

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

1. Introduction

Prediction is inherent to science since it is essential to test theories and their consequences. With modern digital computing, the prediction of natural phenomena represented by mathematical models can now be tested at unprecedented scales.

This digital transformation has led to the emergence of digital twins, which attempt to improve the predictive capability of the models using data. "The aspiration of a digital twin is a close one-to-one mapping between a physical and virtual system", quoting Wagg et al. (2020); which brings enormous challenges, including that of dealing with model verification and validation. The verification of such computational models without reliance on subjectivity is therefore of paramount importance (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)).

According to Razavi et al. (2021), sensitivity analysis methods can be classified in three main approaches: derivative-based, distribution-based, and regression-based, while other approaches (such as variogram-based) are generally a combination of these. Derivative-based approaches compute the derivative of the model functions, either analytically or numerically, and measure the change in the output when the inputs are perturbed around a base point (e.g., see Errico (1997)). 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 alone or in combination with other

inputs (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. For instance, the analytical descriptions 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 their analytical derivation unpractical or difficult. 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 without consensus about these elements. A similar argument can be made for distribution-based methods, which require a precise definition of the probability distributions of model inputs. Regression-based methods require a degree of knowledge of 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 is independent on the model behaviour and requires limited knowledge of input parameters or no additional arbitrary assumptions. This paper presents an interval-based global sensitivity analysis method that fulfills these requirements.

2. Interval Analysis

With interval analysis it is possible to determine the bounds of the output of a function and capture its imprecision. Expressing parameter uncertainties in the form of intervals has the advantage of requiring no assumptions about the uncertainty other than its existence between two bounds, making intervals suitable for modelling epistemic uncertainty.

Interval arithmetic and sampling are the main methods to compute with intervals. 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 meth-

ods, 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 e.g. the Latin Hypercube algorithm, and extracting the minimum and maximum of the outputs of interest (e.g., see 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 (a desirable feature in safety assessments). However, sampling based sensitivity indices can be obtained at not extra cost from the samples used for uncertainty quantification as shown in Plischke et al. (2013) or from inference analysis in Credal Network as in Tolo et al. (2018) .

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 visualisation is a straightforward qualitative method of inspecting dependencies in a model. In this example it is possible to see how y has a linear-like dependence with x_1 (Figure 1 (a)), but shows little or no dependence with x_2 (Figure 1 (b)). The objective is to turn this qualitative *intuition* into a measurement.

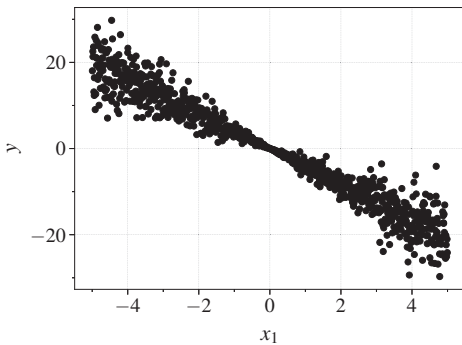
The dependence can be captured measuring the area described by the scatterplot, and comparing it with the box defined by $[y, \bar{y}] \times [x_i, \bar{x}_i]$, where y, \bar{y} are the minimum and maximum of y , and x_i, \bar{x}_i the minimum and maximum of the i^{th} input

parameter. If the measured area equals to the box area, the output has little or no dependence on that input; if the measured area has a value of 0, the output is determined by that input. Any other degree of dependence will fall in-between these two extreme cases.

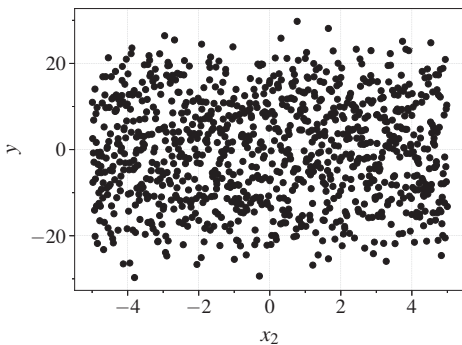
The sensitivity index is calculated with the following formula:

$$S_i = 1 - \frac{\sum_n^N (\underline{x}_i, \bar{x}_i)_n \times (\underline{y}, \bar{y})_n}{(\underline{y}, \bar{y}) \times (\underline{x}_i, \bar{x}_i)}, \quad (1)$$

where N is the total number of subintervals. Therefore, S_i is a sensitivity index ranging from 0 (i.e. y cannot be determined from x_i) to 1 (i.e. y is exactly determined by x_i). Note that the measurement of the output area is an approximation of the actual area, being a consequence of the two different methods employed to solve the model functions: sampling method or subintervalisation.



(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.

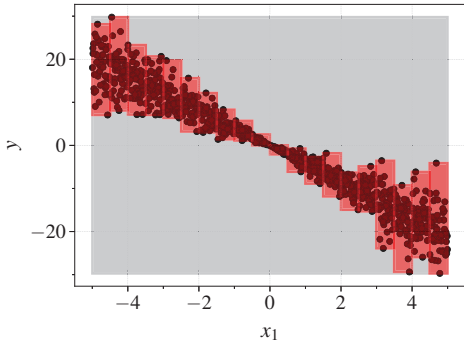
The approximation can be improved increasing the number of samples or subintervals, to the detriment of computational cost.

The area can be calculated with two different methods depending on whether interval arithmetic was employed to calculate the function uncertainty or it was done through 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 computed *for free*. If sampling methods were used, the area can be calculated binning the samples, finding the minimum \underline{y} and maximum \bar{y} in each bin, and calculating the area of each bin. The main drawback of the sampling method is that a step size has to be defined for the binning, and the impact of this parameter on the proposed sensitivity analysis method has not been studied yet.

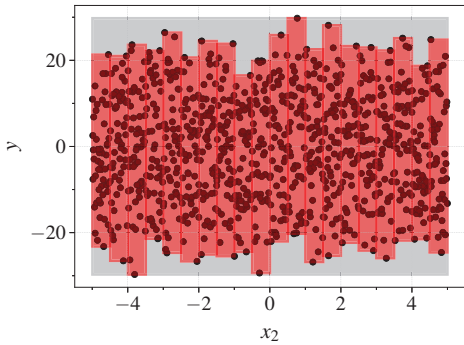
Figure 2 shows the areas calculated with the sampling approach. The algorithm requires the output and input data, and the number of subintervals to divide it. In this example 20 subintervals were used. Then the minimum and maximum output are found for each subinterval, and the area of the rectangle is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

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, 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 can also be seen in Figure 3(b), since the red area equals to the grey area, making $S_2 = 0$), whilst the sampling approach is not as precise. This is caused by the fact that the sampling approach is an inner approximation



(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 .

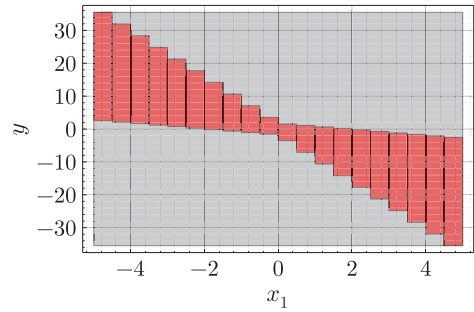
Fig. 2. Results of the evaluation of $y = f(x_1, x_2)$ with $x_1, x_2 \in [-5, -5]$ using 1000 samples generated with Latin Hypercube and 20 subintervals. The sensitivity index is calculated as in Eq. 1, where the numerator is equal to the area coloured in red and the denominator equal to the area coloured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

Table 1. Interval-based sensitivity indices for x_1 (S_1) and x_2 (S_2).

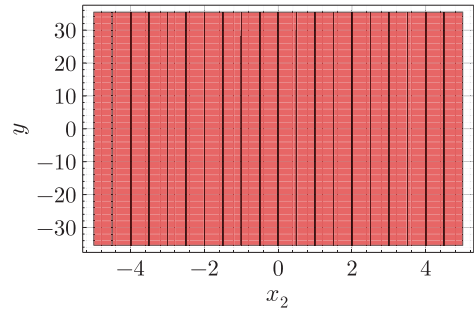
Sensitivity Index	Sampling	Interval arithmetic
S_1	0.790	0.732
S_2	0.197	≈ 0

method, and the greater the number of samples, the more accurate the sensitivity index is.

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



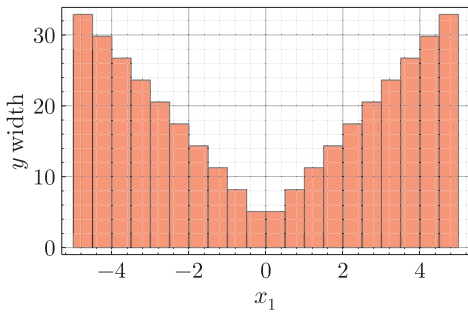
(a) Visualisation of the 20 subintervals of $y = f(x_1, x_2)$ and x_1 .



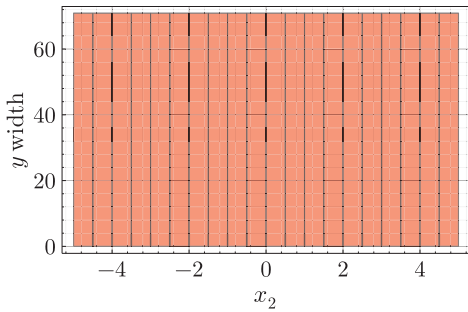
(b) Visualisation of the 20 subintervals of $y = f(x_1, x_2)$ and x_2 .

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.

output uncertainty when the uncertainty of an input is reduced from the interval to a single value (e.g., see Ferson and Tucker (2006); Patelli et al. (2015); 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 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 3 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



(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.

of y depending on the value of x_1 . For example, the best uncertainty reduction is obtained pinching at $x_1 = 0$.

4. Application

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

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

where the constants are set to $a = 5$ and $b = 0.1$, and the input variables x_1, x_2, x_3 are in $[-\pi, \pi]$. 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 .

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 π . 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.

When the inputs of the Ishigami function are independent and uniformly distributed in $[-\pi, \pi]$, the analytical description of the variance terms used to calculate the Sobol’ indices are known; therefore the exact first order and total Sobol’ indices can be calculated in this case. Table 2 contains the analytical Sobol’ indices of the Ishigami function. Analytically, the variance of x_1 is the greatest contributor to the variance of the Ishigami function, and x_3 has effect on the Ishigami only when interacting with x_1 .

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. This example is used to 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 2 shows the results of the analysis. The results suggest that, in this case, the variance of x_2 is the greatest

Table 2. Interval-based and Sobol' sensitivity indices of the Ishigami function. The interval arithmetic based indices were calculated with 100 subintervals. The Sobol' indices for the uniform case were calculated analytically while for the triangular case were calculated with 2048 samples generated with Saltelli sampling.

Sensitivity Index	Interval-based	Uniform distribution		Triangular distribution	
		First Order	Total	First Order	Total
S_1	0.568	0.400	0.711	0.254	0.409
S_2	0.181	0.288	0.288	0.591	0.591
S_3	0.581	≈ 0	0.311	≈ 0	0.158

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.

5. Discussion

When the inputs of the Ishigami function are expressed as intervals, without assuming any distribution function, the interval-based sensitivity analysis claims that x_3 is the most important parameter, since the Ishigami function shows the highest dependence on it, followed by x_1 . Sobol' indices were employed in two different cases of the Ishigami function: one with inputs following a uniform distribution in $[-\pi, \pi]$, and another with inputs were assumed to follow a triangular distribution in $[-\pi, \pi]$ with mode at 0. In the uniform case, x_1 was the first ranked parameter. In the triangular case, x_2 was the first ranked parameter. These results highlight the fact that variance-based methods for sensitivity analysis can return contradictory results when the input distribution function is not accurately known and the variance may not be a reliable statistic.

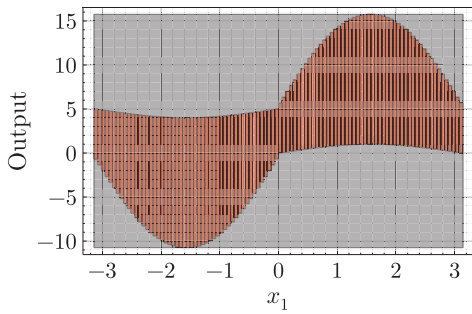
Furthermore, in the context of digital twins it is important not only to perform parameter prioritisation to find on which parameter to focus the uncertainty reduction, but also to find the most effective reduction in output uncertainty. The results from the interval-based approach suggest that, if reducing input uncertainty to a point value were possible, pinching x_1 to $-\pi$, 0, or π would entail the optimum output uncertainty reduction. If reducing to a point value were too restrictive (tech-

nically, economically...), reducing the uncertainty of x_3 from $[-\pi, \pi]$ to $[-1, 1]$ would be the best option. Generally, in variance-based methods the output uncertainty reduction is an average reduction of its variance when the variance of certain input is reduced some % (e.g., see Allaire and Willcox (2012)). In that regard, intervals may be easier to interpret than variances, and therefore the interval-based approach could offer an advantage.

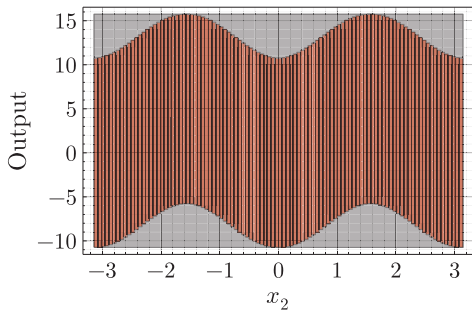
Variance-based methods provide information about interaction effects in the model (as it does with x_1 and x_3), and this is a feature that has not been explored with the interval-based approach. This feature is definitely useful for model diagnostic, and therefore Sobol' indices can be a useful complement to the interval-based approach. Generally, it is desirable to include as many sensitivity analysis methods as possible, as these answer to different questions and can help to better understand the problem under investigation.

6. Conclusion

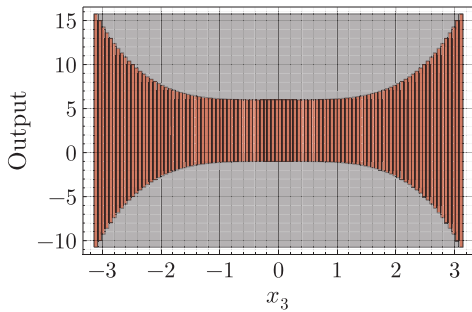
This paper introduces an interval-based method for performing global sensitivity analysis with interval analysis, computed either via sampling method or with interval arithmetic. This method only requires expressing the input parameter uncertainty in the form of intervals, and therefore is particularly suited for cases under epistemic uncertainty. Also, calculating the interval-based sensitivity indices also retrieves all the information of the pinching method, which measures the output uncertainty reduction when input uncertainty is reduced to a point value or subinterval.



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



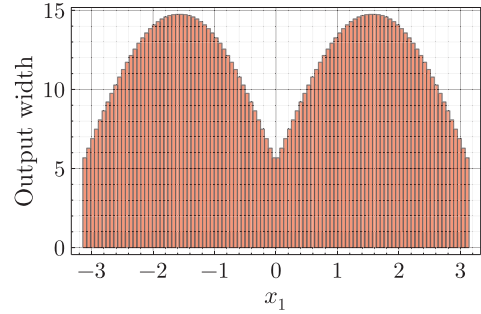
(b) Intervalisation of the Ishigami function and x_2 using 100 subintervals.



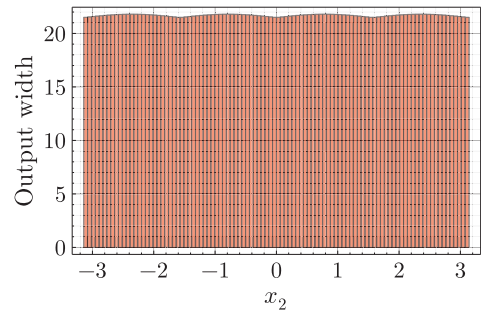
(c) Intervalisation of the Ishigami function and x_3 using 100 subintervals.

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.

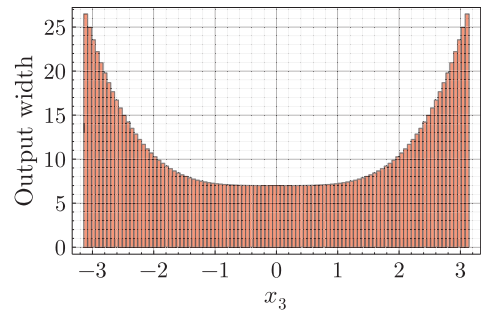
The interval-based approach was applied on the Ishigami function, and its results were compared with the Sobol' indices. The results presented have shown the importance of the knowledge about the probability distribution function of the inputs (i.e. epistemic uncertainty), when variance based methods are used for sensitivity



(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 .

analysis. This effect was illustrated using uniform and triangular distribution functions for the inputs of the Ishigami where the Sobol' indices returned contradictory results when the input distributions were changed. In this respect, when the inputs are not precisely known the interval-based approach is more reliable since it returns the same parameter ranking for a given input domain. This is an

initial work towards sensitivity analysis methods for epistemic uncertainty, and further work should be done to better understand the nature and limitations of the metric presented in this paper.

The code and algorithms used for the production of this document are available in the following repository: <https://github.com/Institute-for-Risk-and-Uncertainty/interval-sensitivity>

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