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PyUncertainNumber for uncertainty propagation with black-box models: beyond probabilistic arithmetic

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Summary

Scientific computations or simulations play a central role in quantifying the performance, reliability, and safety of complex engineered systems. However, these analyses are complicated by the various sources of uncertainties inherent in the computational pipeline. To ensure that complex engineered systems can be operated reliably and robustly even during rare and extreme environment conditions, a comprehensive uncertainty analysis is required. The analysis should be comprehensive in two senses: (i) all possible sources of uncertainty should be identified and represented using approaite mathematical constructs; (ii) The mixture of various types of uncertainties shuold be rigorously propagated through. `pyuncertainnumber` enables such comprehensive analysis, by computing guaranteed bounds on functions of uncertain variables, intrusively and non-intrusively, given only partial empirical knowledge.

Statement of need

A comprehensive uncertainty framework for scientific computation involves a mathematical model, through which various input uncertainties are propagated to estimate the uncertainty of an unknown quantity of interest (QoI). Real world complex systems (physical or engineered) of industrial significance typically involves input parameters subject to uncertainties of various nature (Oberkampf et al., 2004). These input uncertainties are commonly manifested as mixed uncertainties, e.g. probability boxes (p-boxes) which effectively represents a set of distributions, combining both the aleatory and epistemic uncertainty in one structure, or a mixture of uncertainties encompassing, for instance, a vector of inputs parameters of aleatory (e.g. probability distributions), epistemic (e.g. intervals), and mixed nature (e.g. probability boxes).

Probability bounds analysis (Ferson, 2001) is one of the expressive frameworks proposed to manage uncertainties in an imprecise setting (Beer et al., 2013). Software packages have been developed to facilitate the calculations of uncertain quantities, such as interval arithmetic (Angelis, 2022) and probability arithemetic (A. Gray et al., 2021; N. Gray et al., 2022). Collectively, they can be referred to as *uncertainty arithmetic* (Chen & Ferson, 2025) which straightforwardly computes the response provided the performance function.

While it has the potential to automatically compile non-deterministic subroutines via uncertain primitives, its usages face several challenges, one significant challenge is that code accessibility of the simulation model (e.g. finite element or computational fluid dynamics models) of the system is often not guaranteed and hence unable to proceed. This would largely restrict the adoption of mixed uncertainty calculations in real-world applications of computational engineering and physics.

`pyuncertainnumber` addresses this challenge by providing the non-intrusive capability designed to allow generic black-box models to be rigorously propagated with polymorphic uncertainty.

This capability significantly boosts versatility for scientific computations through interfacing with many engineering softwares.

Interval propagation in a non-intrusive manner

Interval analysis (Moore et al., 2009) features the advantages of providing rigorous enclosures of the solutions to problems, especially for engineering problems subject to epistemic uncertainty, such as modelling system paramters due to lack-of-knowledge or characterising measurement incertitude. Naive interval arithmetic typically faces difficulties such as the infamous interval dependency issue. Though it may be mitigated through arithmetic rearrangements in some simple cases, it still can challenging for models of most complex systems. The critical issue remains the accessibility of code.

Generally, the interval propagation problem can be cast as an optimisation problem where the minimum and maximum are sought via a function mapping. The function, for example f in Equation 1, is not necessarily monotonic or linear and may well be a black-box deterministic model for a generic system.

$$Y = f(I_{x1}, I_{x2}, ..., I_{xn}) \tag{1}$$

where $\mathbf{I} = [\underline{\mathbf{I}}, \overline{\mathbf{I}}] = [I_{x1}, I_{x2}, ..., I_{xn}]^{\mathsf{T}}$ represents the vector of interval-valued inputs. For black box models the optimisation can generally be solved via gradient-free optimisation techniques.

$$\underline{Y} = \min_{\underline{\mathbf{I}} \leq \mathbf{I} \leq \overline{\mathbf{I}}} [f(\mathbf{I})]; \ \overline{Y} = \max_{\underline{\mathbf{I}} \leq \mathbf{I} \leq \overline{\mathbf{I}}} [f(\mathbf{I})]$$

`pyuncertainnumber` provides a series of non-intrusive methodologies of varying applicability. It should be noted that there is generally a trade-off between applicability and computational efficiency. With more knowledge pertaining the characteristics of the underlying function, one can accordinly dispatch an efficient method. For example, when monotonicity is known one can use the vertex method which requres 2^n model evaluations. Furthermore, the accuracy of these methods varies, and a common rule of thumb indicates that increasing the number of model evaluations generally leads to improved accuracy. A summary of applicability is tabulated in Table 1, readers can refer to (Chen & Ferson, 2025) for additional details.

Table 1: Supported methods for non-intrusive interval propagation.

Method	End-points	Subinterval reconstitution	Cauchy-Deviate method	Bayesian optimisation	Genetic algorithm
Assumption	monotonicity	monotonicity in subinterlvas	linearity and gradient required	No	No
Example result	[13.0,148.0]	[13.0,148.0]	[-11.7,100.67]	[13.0,148.0]	[13.0,147.8]

To better demonstrate the non-intrusive capability, two numerical examples, as displayed below in Figure 1, are provided where they are treated as black-box models. Table 1 lists the response interval of $f_b([1,5],[7,13],[5,10])$ for respective methods.

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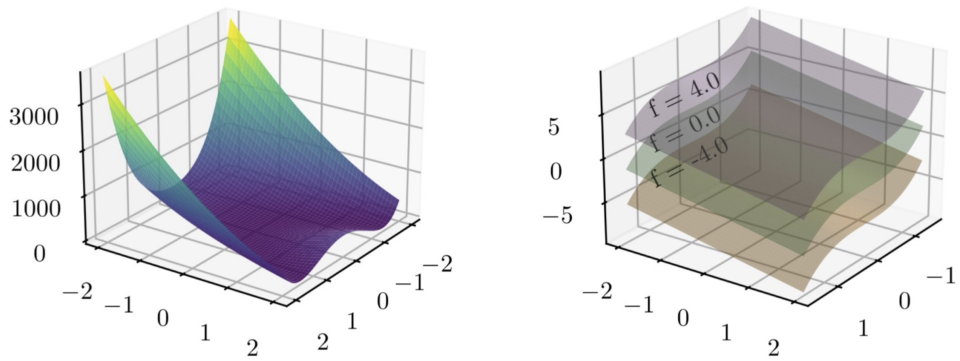

(a) (b)

Figure 1: Exampler functions as black-box models. (a) $f_a(x, y) = 100(x - y^2)^2 + (1 - x)^2$; (b) $f_b(x, y, z) = x^3 + y + z$

Mixed uncertainty propagation for black-box models

Real world complex systems (physical or engineered) of industrial significance typically involves parameters subject to uncertainties of various nature (Oberkampf et al., 2004). It requires faithful characterisation of these uncertainties given the empirical information, and the approaach to rigorously progate them. Due to the fact that empirical information is often sparse or scarce or conflicting, even the uncertainty characterisation for one parameter could be of mixed nature, for example one may be confident about the distributional family but uncertain about its shape parameters, or when there exists multiple expert opiontion of different credibility regarding its elicitation. Commonly, real systems expect a high-dimensional input which effectively represents a mixture of aleatory, epistemic, and mixed uncertainties, as symbolfied below:

$$Y = f(\mathbf{u}; C) \tag{2}$$

where $\mathbf{u} \in \mathbb{R}^n$ denotes the collection of n uncertain inputs and C denotes intervariable dependency structure.

When both aleatory and epistemic uncertainties are present in $\mathbf{u}$, a *nested (double) Monte Carlo* approach can be used for determininsitc models without confounding the two distinct types of uncertainty. As illustrated in Figure 2, Latin-hypercube samples are first drawn from the epistemic interval, conditioned on which aleatory samples are drawn from the aleatoric probability distributions. Propagate these samples, which are visually denoted as rug ticks alongside the abscissa, through the computational model results in an ensemble of CDF (cumulative distribution function) of the QoI whereby a final p-box is obtained as the envelope. Each CDF (orange color) correponds to an epistemic sample.

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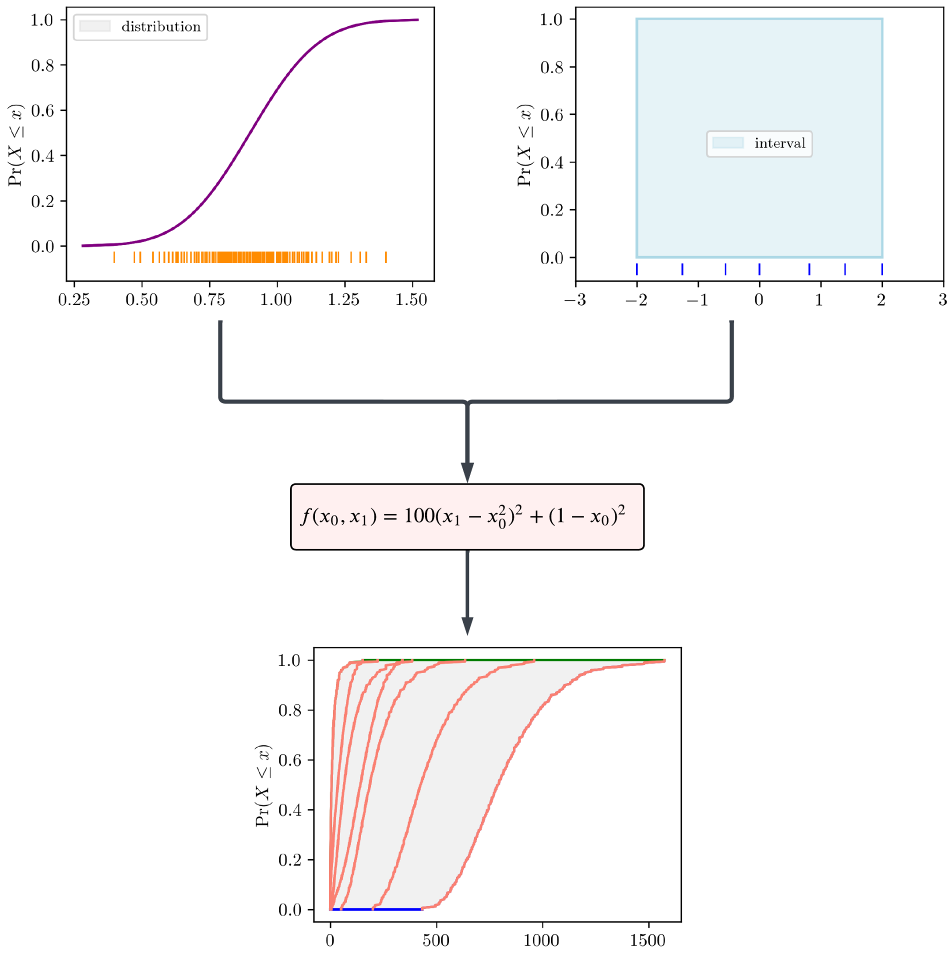

Figure 2: Workflow of the Double Monte Carlo method.

To scale to a more realistic setting, Figure 3 illustrates the workflow of *interval Monte Carlo* method where a mixture of aleatory, epistemic, and mixed uncertainty parameters are present, and a certain copula is specified denoting the dependency structure. Correlated samples in the uniform space from the copula, visually denoted as rug ticks alongside the probability axis, are converted to physical space through alpha-cuts. Interval propagation (see the last section) then does the heavy lifting in which scalar values can be considered as degenerate intervals. As a result, the response QoI in Figure 3 is then obtained as a p-box shown in gray. In contrast, a pinched response, obtained from propagating pinched input variables (e.g. a p-box is pinched into a distribution and an interval is pinched into a scalar), is also shown as a comparison. Importantly, the pinched result being enclosed in the p-box manifests a critical feature of probability bounds analysis which yields results that are guaranteed to encolse all possible distributions of the ouput so long as the input p-boxes were all sure to enclose their respective distributions.

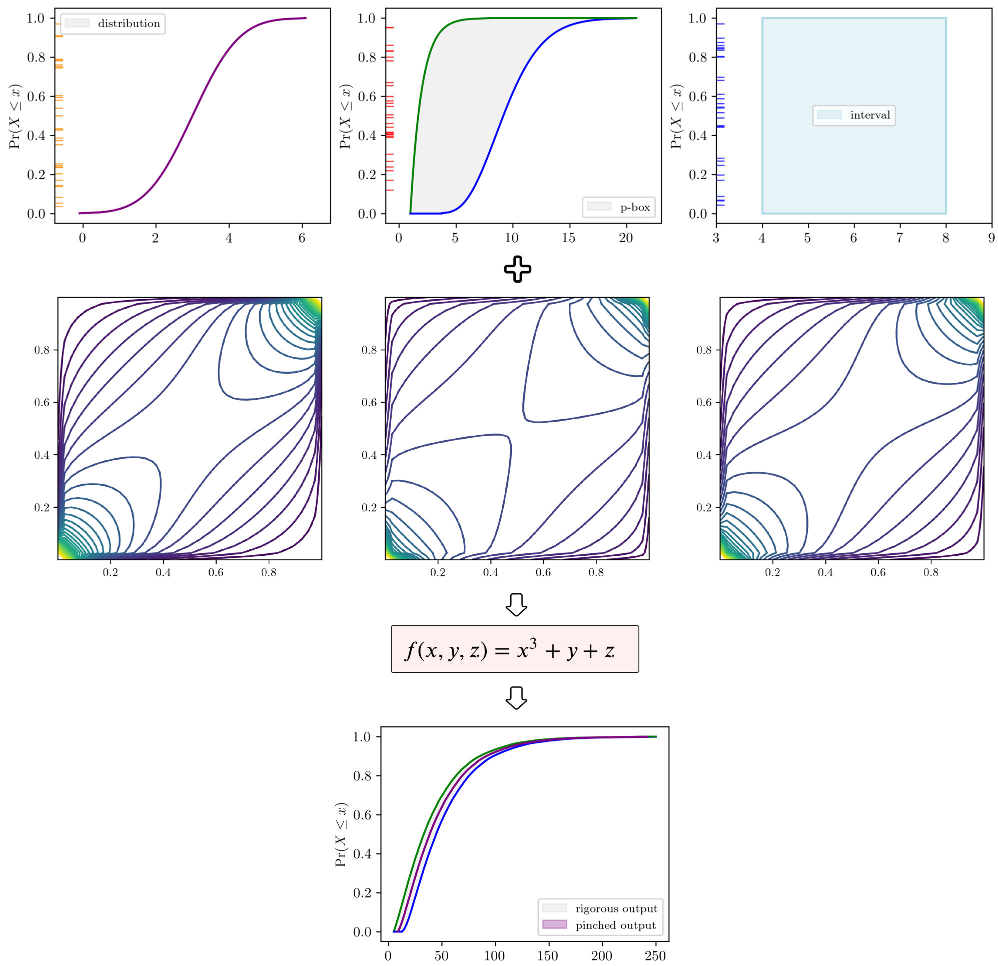

Figure 3: Workflow of the Interval Monte Carlo method. The first row shows the marginal of the inputs and the second row shows the bivariate copula density.

Conclusion

It is evident that many computational tasks in engineering and physics rely on complex numerical methods in which the model functions are black boxes. This makes uncertainty arithmetic difficult to cope due to the code accessibility of models. By providing methods supporting generic black box models, `pyuncertainnumber` enables rigorous uncertainty analysis for real-world scenarios of mixed uncertainties and partial knowledge. This non-intrusive capability allows `pyuncertainnumber` to interface with multiple software environments to provide extensive compatibility with engineering applications, thereby its applicability across diverse computational workflows.

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