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

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Summary

Scientific calculations and simulations are complicated by various uncertainties inherent in the computational pipeline. Comprehensive analysis requires uncertainties be represented using mathematical constructs that distinguish variability from lack of knowledge and combine them rigorously in calculations. The new Python library `pyuncertainnumber` enables such analysis by computing guaranteed bounds on functions of uncertain variables given only partial empirical knowledge. It supports both intrusive methods that are efficient for projection through explicitly defined mathematical models and non-intrusive methods that can be used with black-box models that associate outputs with given inputs but whose internal workings are not known.

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; Smith, 2024). These input uncertainties often appear as a mixture of parameters subject to variability (i.e. aleatory uncertainty, typically represented by probability distributions), or lack of knowledge (i.e. epistemic uncertainty, often represented by intervals), or a combination of both (i.e. mixed uncertainty, often represented by probability boxes (p-boxes)), which effectively represent a set of distributions and thereby capture both aleatory and epistemic uncertainty within a unified structure.

Probability bounds analysis (Ferson, 2001; Springer, 1979; Williamson & Downs, 1990) 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 *probabilistic arithmetic* (A. Gray et al., 2021; N. Gray et al., 2022). Collectively, they can be referred to as *uncertainty arithmetic* (Chen & Ferson, 2025), which provides a straightforward way to compute outcomes from algebraic expressions involving uncertain variables.

While these uncertainty-representing frameworks have the potential to automatically compile non-deterministic subroutines via uncertain primitives, their use faces several challenges. A major one is that code accessibility[1] of the simulation models or software (e.g. finite-element or computational-fluid-dynamics models) employed to describe the behavior of the system is often not guaranteed, rendering intrusive[2] use of the above-mentioned uncertainty-representing frameworks infeasible. Often, these models are treated as black-box models in practice. Consequently, there is a critical need for software tools capable of performing mixed-uncertainty

[1] access to the source code.
[2] requiring access or modification of the source code of a computational model.

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calculations on black-box models in real-world applications of computational engineering and physics.

pyuncertainnumber addresses this need by providing the non-intrusive[3] capability designed to allow generic black-box models to be rigorously propagated in the face of mixed uncertainties. This capability significantly boosts versatility for scientific computations through interfacing with many engineering software whose internal workings are not known.

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 parameters 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 be challenging for models of most complex systems, and impossible for black-box models. 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 of the response are sought given a function mapping. Consider the function, for example f in Equation 1, which 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 $\mathbf{I} = [\underline{\mathbf{I}}, \overline{\mathbf{I}}] = [I_{x1}, I_{x2}, ..., I_{xn}]^{\mathrm{T}}$ represents the vector of interval-valued inputs. For black-box models the optimisation can generally be solved via gradient-free optimisation techniques, as shown below:

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

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 additional knowledge pertaining the characteristics of the underlying function, one can accordinly dispatch an efficient method. For example, if the function is known to be monotone, one may employ the vertex method (Dong & Shah, 1987) which requres only 2^n model evaluations and is therefore subtantially more efficient than a brute-force grid sampling scheme. It should be noted that the accuracy of these methods varies, and a common guideline is that increasing the number of model evaluations generally leads to a better estimate of the bound but at the cost of compututational burden. A summary of applicability is tabulated in Table 1; see Chen & Ferson (2025) for additional details of their advantages and disadvantages.

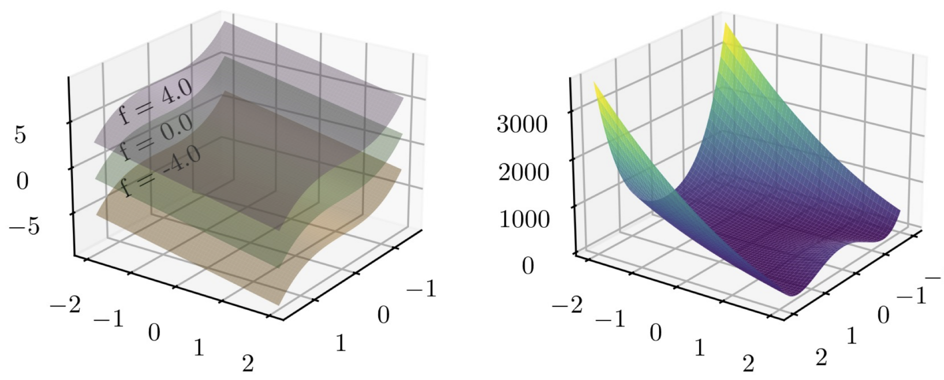
Table 1: Supported methods for non-intrusive interval propagation.

Category	Assumption	Results of Example A
Vertex (Endpoints)	monotonicity	[13.0,148.0]
Subinterval reconstitution	monotonicity in subintervals	[13.0,148.0]
Cauchy-deviate method	linearity and gradient required	[-11.7,100.67]
Bayesian optimisation	general applicability	[13.0,148.0]

[3] operating on the model as a black box, without accessing or modifying its internals.

Category	Assumption	Results of Example A
Genetic algorithm	general applicability	[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 $f_a([1,5],[7,13],[5,10])$ for respective methods. A reference ground truth is $[13.0, 148.0]$.



(a) (b)

Figure 1: Examplar functions as black-box models. (a) Example A: $f_a(x,y,z) = x^3 + y + z$, three level sets of $f_b = 4$, $f_b = 0$, $f_b = -4$ are shown; (b) Example B: $f_b(x,y) = 100(x-y^2)^2 + (1-x)^2$.

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 with the examplar function B (see Figure 1), 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.

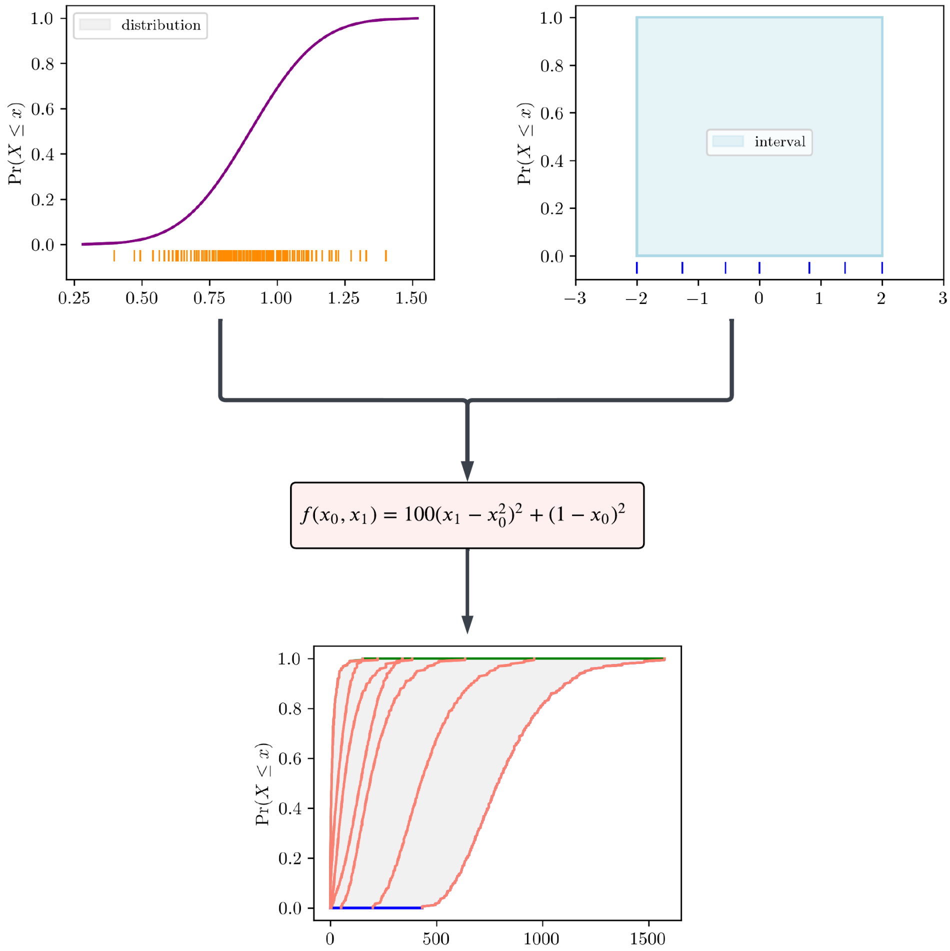


Figure 2: Workflow of the Double Monte Carlo method.

To scale to a more realistic setting, Figure 3 illustrates the workflow of *interval Monte Carlo* method using the examplar function A where a mixture of aleatory, epistemic, and mixed uncertainty parameters are present, plus 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.

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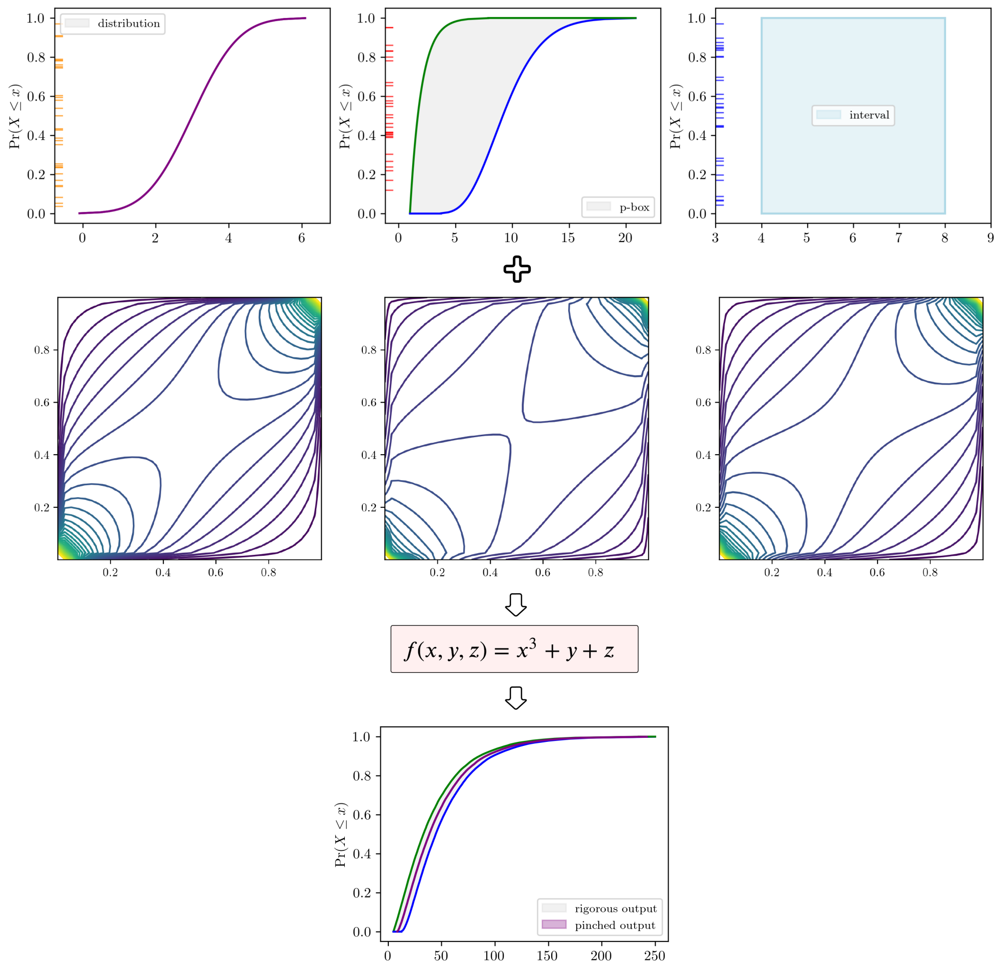

Figure 3: Workflow of the Interval Monte Carlo method. The first row shows the marginal of the inputs and the second row shows the bivariate copula density.

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 manage because the model code is inaccessible. 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, offering extensive compatibility with engineering applications and diverse computational workflows.

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