

# Numerical approach for quantification of epistemic uncertainty

John Jakeman<sup>a</sup>, Michael Eldred<sup>b,1</sup>, Dongbin Xiu<sup>c,\*,2</sup>

<sup>a</sup> Department of Mathematics, Australian National University, Australia

<sup>b</sup> Sandia National Laboratories, Albuquerque, NM 87185, United States

<sup>c</sup> Department of Mathematics, Purdue University, West Lafayette, IN 47907, United States

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## ABSTRACT

In the field of uncertainty quantification, uncertainty in the governing equations may assume two forms: aleatory uncertainty and epistemic uncertainty. Aleatory uncertainty can be characterised by known probability distributions whilst epistemic uncertainty arises from a lack of knowledge of probabilistic information. While extensive research efforts have been devoted to the numerical treatment of aleatory uncertainty, little attention has been given to the quantification of epistemic uncertainty. In this paper, we propose a numerical framework for quantification of epistemic uncertainty. The proposed methodology does not require any probabilistic information on uncertain input parameters. The method only necessitates an estimate of the range of the uncertain variables that encapsulates the true range of the input variables with overwhelming probability. To quantify the epistemic uncertainty, we solve an *encapsulation problem*, which is a solution to the original governing equations defined on the estimated range of the input variables. We discuss solution strategies for solving the encapsulation problem and the sufficient conditions under which the numerical solution can serve as a good estimator for capturing the effects of the epistemic uncertainty. In the case where probability distributions of the epistemic variables become known *a posteriori*, we can use the information to post-process the solution and evaluate solution statistics. Convergence results are also established for such cases, along with strategies for dealing with mixed aleatory and epistemic uncertainty. Several numerical examples are presented to demonstrate the procedure and properties of the proposed methodology.

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## 1. Introduction

Mathematical models are used to simulate a wide range of systems and processes in engineering, physics, biology, chemistry and environmental sciences. These systems are subject to a wide range of uncertainties. The effects of such uncertainty should be traced through the system thoroughly enough to allow one to evaluate their effects on the intended use of the model usually, but not always, related to prediction of model outputs.

There are two forms of model uncertainty: aleatory and epistemic. Aleatory uncertainty arises from the inherent variation associated with the system under consideration and is irreducible. Epistemic uncertainty represents any lack of knowledge

\* Corresponding author. Tel.: +1 765 496 2846.

E-mail addresses: [john.jakeman@anu.edu.au](mailto:john.jakeman@anu.edu.au) (J. Jakeman), [mseldre@sandia.gov](mailto:mseldre@sandia.gov) (M. Eldred), [dxiu@purdue.edu](mailto:dxiu@purdue.edu) (D. Xiu).

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or information in any phase or activity of the modeling process [13] and is reducible through the introduction of additional information.

The sources of aleatory uncertainty are typically represented using a probabilistic framework under which the aleatory uncertainty can be represented by a finite number of random variables with some known distribution. The sources of aleatory uncertainty include both uncertainty in model coefficients (parametric uncertainty) and uncertainty in the sequence of possible events (stochastic uncertainty). Stochastic uncertainty is entirely aleatory by nature. Parametric uncertainty can also be completely aleatory if the complete distribution of all the model parameters are known *a priori*.

Frequently, strong statistical information such as probability distribution functions or high-order statistical moments is not available. Experimental data needed to construct this information is often expensive and consequently no data, or only a small collection of data points, may be obtainable. In these cases “expert opinion” is used in conjunction with the available data to produce weak inferential estimates of parametric characteristics, often in the form of lower and upper bounds. Other sources of epistemic uncertainty include limited understanding or misrepresentation of the modeled process, known commonly as “model form” uncertainty. Inclusion of “enough” additional information about either the model parameters or structure can lead to a reduction in the predicted uncertainty of a model output. Consequently, we can consider epistemic uncertainty as providing (conservative) bounds on an underlying aleatory uncertainty, where reduction and convergence to the true aleatory uncertainty (or, in some cases, a constant value) can be obtained given sufficient additional information.

Until recently, most uncertainty analysis has focused on aleatory uncertainty. Numerous methods have been developed that provide accurate and efficient estimates of this form of uncertainty. In particular, stochastic Galerkin (SG) [2,9,28] and stochastic collocation (SC) [1,5,8,16,21,25,27] methods provide accurate representations of aleatory uncertainty and have the ability to deal with steep non-linear dependence of the solution on random model data. For a detailed review on the methods, see [26].

In comparison to the quantification of aleatory uncertainty, the analysis of epistemic uncertainty has proved more challenging. Probabilistic representations of epistemic uncertainty are inappropriate, since the characterization of input epistemic uncertainty through well-defined probability distributions imposes a large amount of unjustified structure on the influence of the inputs on the model predictions. This can result in stronger inferences than are justified by the available data. Evidence theory [12], possibility theory [4] and interval analysis [11,19] have been proposed as more appropriate alternatives, where they are listed in descending order based on the amount of imposed input structure.

Of the aforementioned methods, evidence theory is the most closely related to probability theory. Evidence theory starts from basic probability assignments on the inputs, propagates these descriptions through a model using standard sampling techniques, and produces estimates of the lowest and highest probabilities of the model observables. These estimates define cumulative belief and cumulative plausibility functions that represent the uncertainty in the output metrics, where belief provides a measure of the amount of information that supports an event being true and plausibility measures the absence of information that supports the event being false. The evidence theory representation of uncertainty approaches the probabilistic representation as the amount of information about the input data increases [12].

Possibility theory is closely related to fuzzy set theory and, similar to evidence theory, utilizes two descriptions of likelihood, necessity and possibility. These two measures are based upon the properties of individual elements of the universal set of events, unlike plausibility and belief which are derived from the properties of subsets of the universal set. For more details, see [10].

Evidence and possibility theory require aggregation of data from multiple sources into a format consistent with the chosen technique. In practice, this can be difficult and time consuming. Interval analysis [17], on the other hand, only requires upper and lower bounds on the uncertain input data. Sampling and/or optimization [5,19] is then used to generate upper and lower bounds (intervals) on the model outputs from predefined intervals on the input data.

The application of evidence theory, possibility theory and interval analysis to non-linear and complex problems often requires a prohibitively large number of samples and typically underestimates the output extrema. Global surrogate models have been used in an attempt to alleviate this problem [10]; however, the performance of these approaches is highly dependent on the accuracy of the surrogate model and construction costs can be high when global accuracy is required and convergence rates are not exponentially fast. In more recent work, surrogates with adaptive refinement strategies have been combined with stochastic collocation methods [5,6,19,20] in order to segregate aleatory quantification with stochastic expansions from epistemic quantification using optimization-based interval estimation.

The choice of the aforementioned methods depends on the amount of available information which can be utilized to characterize the input uncertainty. Consequently this choice is highly problem dependent. Here we propose a new and more general framework to numerically quantify epistemic uncertainty. This proposed method can deal with varying amounts of information on the input data from simple bounds to full probabilistic descriptions, and thus can seamlessly handle the problems with both epistemic and aleatory uncertainties. Furthermore the proposed approach utilizes the classical approximation theory in multi-dimensional space and achieves high efficiency than the methods currently available.

Unlike many existing numerical methods for quantifying epistemic uncertainty, the proposed method requires only an approximation of the ranges of the input data that encapsulates the “true” bounds of the input data. We then propose solving an “encapsulation problem” which generates a solution to the governing equations in a domain that encloses the true (and unknown) probability space. Here a multi-dimensional polynomial expansion can be employed to approximate the solution on the larger encapsulation space. We show that if such a representation converges in the encapsulation space then this method will also converge in the true probability space. Furthermore, convergence is maintained even in the presence of

dependencies between input data. We also demonstrate numerically that if the distributions of the input data are found *a posteriori*, the polynomial approximation of the solution statistics will converge.

In Section 2, we present the necessary mathematical framework for quantifying epistemic uncertainty and in Section 3 we discuss the construction and solution of the encapsulation problem. In particular we focus on polynomial based Galerkin and collocation methods and illustrate how these methods can be used to construct efficient and accurate approximations of the solution to the encapsulation problem. We also extend the encapsulation approach to models with mixed epistemic and aleatory uncertainty and discuss how to extract and interpret important statistical information. Numerical examples are presented in Section 4 and we conclude the paper in Section 5.

## 2. Problem setup

Let  $D \subset \mathbb{R}^\ell$ ,  $\ell = 1, 2, 3$ , be a physical domain with coordinates  $x = (x_1, \dots, x_\ell)$  and let  $T > 0$  be a real number. We consider the following general stochastic partial differential equation

$$\begin{cases} v_t(x, t, Z) = \mathcal{L}(v), & D \times (0, T] \times I_Z, \\ \mathcal{B}(v) = 0, & \partial D \times [0, T] \times I_Z, \\ v = v_0, & D \times \{t = 0\} \times I_Z, \end{cases} \quad (2.1)$$

where  $\mathcal{L}$  is a (non-linear) differential operator,  $\mathcal{B}$  is the boundary condition operator,  $v_0$  is the initial condition, and  $Z = (Z_1, \dots, Z_d) \in I_Z \subset \mathbb{R}^d$ ,  $d \geq 1$ , are a set of random variables characterizing the random inputs to the governing equation. The solution is therefore a stochastic quantity,

$$v(x, t, Z) : \bar{D} \times [0, T] \times I_Z \rightarrow \mathbb{R}^{n_v}. \quad (2.2)$$

Without loss of generality, hereafter we assume (2.1) is a scalar system with  $n_v = 1$ . We also make a fundamental assumption that the problem (2.1) is well-posed in  $I_Z$ .

Most of the existing studies adopt a probabilistic formulation to quantify *aleatory* uncertainty. That is, it is typically assumed that the distribution of the random variables  $Z$  is known, with the most widely adopted approach assuming the marginal distributions of  $Z_i$  are known and all  $Z_i$  are independent from each other. In this paper, however, we consider the case where the uncertainty is *epistemic*. That is, the distribution functions of  $Z_i$  are not known, primarily due to our lack of understanding and characterization of the physical system governed by the system of equations (2.1).

The focus is on the dependence of the solution on the uncertain inputs  $Z$ ; therefore, we present solutions for fixed location  $x$  and time  $t$  and omit these variables whenever possible.

## 3. Methodology

We now present a method for solving system (2.1) subject to epistemic uncertain inputs. The proposed methodology is a three-step procedure which involves identifying the ranges of the uncertain inputs, generating an accurate polynomial approximation of the solution to (2.1) within estimated ranges and post-processing the results. Note that no probability distribution information will be utilized in the solution procedure.

### 3.1. Range estimation

Unlike traditional aleatory uncertainty quantification, the proposed method only requires an estimate of the ranges of the random input.

The goal is to identify a range, or bound, that is sufficiently large such that the “true”, and yet unknown, range of the input uncertainty is *mostly* incorporated. We now illustrate the idea more precisely.

For each random variable  $Z_i$ ,  $i = 1, \dots, d$ , let

$$I_{Z_i} = [\alpha_i, \beta_i], \quad \alpha_i < \beta_i, \quad (3.1)$$

be its (unknown) support. We consider the following two cases.

- *Bounded*: That is,  $I_{Z_i}$  is a bounded interval with

$$-\infty < \alpha_i < \beta_i < \infty.$$

- *Unbounded*: That is, either

$$\alpha_i = -\infty \quad \text{and/or} \quad \beta_i = \infty.$$

This implies that the distribution of  $Z_i$  has tail(s) near infinity.

The goal of range estimation is to identify a bounded interval

$$I_{X_i} = [a_i, b_i], \quad -\infty < a_i < b_i < \infty, \tag{3.2}$$

such that  $I_{X_i}$  and  $I_{Z_i}$  overlap each other with sufficiently large probability. Let us consider the symmetric difference between  $I_{X_i}$  and  $I_{Z_i}$ , i.e.,

$$I_i^- = I_{Z_i} \triangle I_{X_i} = (I_{Z_i} \cup I_{X_i}) \setminus (I_{Z_i} \cap I_{X_i}). \tag{3.3}$$

We then require the range  $I_{X_i}$  is defined in (3.2) such that, for a small real number  $\delta_i \geq 0$ ,

$$P(Z_i \in I_i^-) \leq \delta_i. \tag{3.4}$$

Intuitively speaking, this requires the tail probability of  $Z_i$ , if there is any, outside the bounded interval  $I_{X_i}$  to be sufficiently small. It can always be achieved by choosing the  $I_{X_i}$  sufficiently wide. If  $I_{Z_i}$  is bounded then we can always choose  $I_{X_i}$  to overlap  $I_{Z_i}$  completely. In such a case,  $I_{Z_i} \subseteq I_{X_i}$  and  $P(Z_i \in I_i^-) = 0$ .

Note the proposed method removes the need for accurate estimates of the input ranges. The estimate of the range must ensure that the range be sufficiently wide such that it encapsulates the “true” input range either completely if the “true” range is bounded, or with overwhelming probability if the “true” range is unbounded. The specific techniques for range estimation is not the focus of this paper and will be left for another time.

In addition to ensuring the *encapsulation condition* (3.4) is satisfied one must also ensure that the governing equations (2.1) are well-posed in the region of  $I_{X_i}$ . That is, the “over-estimation” part of the  $I_{X_i}$ ,  $I_{X_i} \cap I_i^-$ , does not pose any problem for the solution of (2.1). Consequently the properties of the system (2.1) must be used to guide the range estimation procedure.

### 3.2. Encapsulation problem

Let  $I_Z$  be the range of the random variables  $Z \in \mathbb{R}^d$ . Naturally,

$$I_Z \subseteq \times_{i=1}^d I_{Z_i}. \tag{3.5}$$

We also define an *encapsulation set*

$$I_X = \times_{i=1}^d I_{X_i} = \times_{i=1}^d [a_i, b_i]. \tag{3.6}$$

which is the Cartesian product of (3.2). Now let

$$I^+ = I_Z \cup I_X, \quad I^o = I_Z \cap I_X, \tag{3.7}$$

and

$$I^- = I_Z \triangle I_X = I^+ \setminus I^o, \tag{3.8}$$

be the symmetric difference of  $I_Z$  and  $I_X$ . By following the construction of the range estimate in (3.3) and (3.4), it is easy to see that

$$P(Z \in I^-) \leq \delta, \quad \delta = \delta_i^d. \tag{3.9}$$

Therefore, the encapsulation set  $I_X$  encapsulates  $I_Z$ , the “true” and unknown support of  $Z$ , with probability at least  $1 - \delta$ , where  $\delta \geq 0$  can be made small by enlarging the size of  $I_X$ . The parameter  $\delta$  can be zero, i.e.,  $I_X$  encapsulates  $I_Z$  with probability one, when  $I_Z$  is a bounded domain.

We now define the following *encapsulation problem*

$$\begin{cases} u_t(x, t, X) = \mathcal{L}(u), & D \times (0, T] \times I_X, \\ \mathcal{B}(u) = 0, & \partial D \times [0, T] \times I_X, \\ u = u_0, & D \times \{t = 0\} \times I_X, \end{cases} \tag{3.10}$$

where  $I_X$  is the bounded hypercube defined in (3.6). This is effectively the same problem (2.1) defined now on the encapsulation set  $I_X$  that covers the original random parameter set  $I_Z$  with probability at least  $1 - \delta$ . The new problem is well defined in  $I_X$  because we have assumed the estimated range of each  $I_{X_i}$  stays in the range of well-posedness allowed by the governing equation. Since problem (2.1) and (3.10) are exactly the same in the common domain  $I^o$ , we have the following trivial result,

$$u(\cdot, \xi) = v(\cdot, \xi), \quad \forall \xi \in I^o. \tag{3.11}$$

We remark that for the *encapsulation problem* (3.10) we do not assign any probability information to variables  $X$ .

### 3.3. Solution for the encapsulation problem

For solution of the encapsulation problem (3.10), we again focus only on the dependence on the variables  $X$ , which now resides in the hypercube  $I_X \subseteq \mathbb{R}^d$ .

For any fixed location  $x$  and time  $t$ ,

$$u(X) : I_X \rightarrow \mathbb{R}. \tag{3.12}$$

A critical requirement for the proposed methodology is the need for the numerical approximation of (3.10) to converge point-wise. Let  $u_n(X)$  be a numerical solution, where the index  $n$  is associated with discretization parameters used in the approximation. We then require

$$\epsilon_n \triangleq \|u - u_n\|_{L^\infty(I_X)} \rightarrow 0, \quad n \rightarrow \infty, \tag{3.13}$$

where  $\|\cdot\|_\infty$  is the standard  $L^\infty$  norm defined as

$$\|u\|_{L^\infty(I_X)} = \sup_{X \in I_X} |u(X)|.$$

When  $u$  is sufficiently smooth, such kind of point-wise convergent approximation can be obtained, at least in principle.

While there are choices for solving the encapsulation problem (3.10), here we will focus on polynomial approximation  $u_n$ , where the index  $n$  is typically associated with the highest degree of polynomials used in the approximation. This kind of methods are direct extension of polynomial approximation theory and the generalized polynomial chaos (gPC) methods used primarily for aleatory uncertainty analysis. Again we emphasize that the key of choosing a particular method is that, despite its computational efficiency, it should provide an accurate approximation in the  $L^\infty$  norm of (3.13).

Without loss of generality and merely for notational convenience, hereafter we assume the encapsulation set  $I_X$  is a hypercube

$$I_X = [-1, 1]^d, \quad d \geq 1. \tag{3.14}$$

Note this can always be accomplished by properly translating and scaling of the variables  $X$  in (3.10).

### 3.3.1. Collocation approach

The solution  $u(X)$  to the encapsulation problem (3.10) is decoupled in the parameter space  $I_X$ . Subsequently we can solve (3.10) at a set of discrete nodes and then construct a polynomial approximation of  $u$  that interpolates the solution at each node. This so called collocation approach has been used extensively to quantify aleatory uncertainty [1,25,27]

Let  $\Theta_n = \{X^j\}_{j=1}^m \subset I_X$  be a set of (prescribed) nodes, where  $m \geq 1$  is the number of nodes. By adopting the collocation methodology, we enforce (3.10) at the node  $X^j$ ,  $j = 1, \dots, m$ , and solve

$$\begin{cases} u_t(x, t, X^j) = \mathcal{L}(u), & D \times (0, T], \\ \mathcal{B}(u) = 0, & \partial D \times [0, T], \\ u = u_0, & D \times \{t = 0\}. \end{cases} \tag{3.15}$$

It is easy to see that for each  $j$ , (3.15) is a deterministic problem with fixed values of  $X$ . Therefore, solving the system poses no difficulty provided one has a well-established deterministic algorithm.

Let  $u^j = u(\cdot, X^j)$ ,  $j = 1, \dots, m$ , be the solution of the above problem and  $\{u^j\}_{j=1}^m$  be the ensemble of solutions obtained by solving (3.15). Through use of the solution ensemble, we then seek to construct  $u_n(X) \in \Pi(X)$ , where  $\Pi(X)$  is a proper polynomial space, so that the convergence property (3.13) can be achieved.

While the general strategy is straightforward, the options for practical implementation are limited. Multivariate approximation is a challenging area with many open issues. Here, we describe a more established method based on sparse grid interpolation [3], which has been used extensively in quantifying aleatory uncertainty following the work of [27].

Sparse grid interpolation, is based upon a combination of one-dimensional interpolation formula. Let  $\Theta_1^i = \{X_1^1, \dots, X_1^{m_i}\}$  be a set of distinct nodes in the direction  $X_i$  and  $\{u(X_1^j)\}_{j=1}^{m_i}$  the numerical solution at these nodes. We can approximate the one-dimensional component of the solution  $u$  over the range of  $X_i$  using the following interpolation formula

$$\mathcal{U}_i[u] = \sum_{j=1}^{m_i} u(X_1^j) \cdot \Psi_i^j(X_i), \tag{3.16}$$

where  $m_i$  is the number of collocation nodes and  $\Psi_i^j$  is the interpolating basis which satisfies the discrete orthogonality property  $\Psi_i^j(X_1^k) = \delta_{jk}$ . The Lagrange polynomials and the piecewise linear basis are two commonly used bases.

In the multivariate case  $d > 1$  we can approximate  $u$  by the  $N$ th-level Smolyak formula ([18])

$$u_N = \sum_{N-d+1 \leq |\mathbf{i}| \leq N} (-1)^{N-|\mathbf{i}|} \cdot \binom{d-1}{N-|\mathbf{i}|} \cdot (u_{i_1} \otimes \dots \otimes u_{i_d}), \tag{3.17}$$

where  $\mathbf{i} = (i_1, \dots, i_d)$  and  $|\mathbf{i}| = i_1 + \dots + i_d$ . See [24] for detailed derivation of the formula. To compute the interpolating solution

$$u_N(X) = \mathcal{U}_N[u],$$

one only needs to evaluate the function  $u$  on the *sparse grid*,

$$H_{N,d} = \bigcup_{N-d+1 \leq |i| \leq N} (\Theta_1^{i_1} \times \dots \times \Theta_1^{i_d}). \tag{3.18}$$

To achieve better efficiency, the nodal sets should be nested so that  $\Theta^i \subset \Theta^{i+1}$  and  $H_{N,d} \subset H_{N+1,d}$ . This means that to increase the level of interpolation from  $N$  to  $N + 1$  we need only solve (3.10) on the new set of points  $H_{N+1,d} \setminus H_{N,d}$ .

Unlike a full tensor product construction, which suffers from the *curse of dimensionality* in that the number of nodes grows exponentially with the dimension  $d$ , the number of nodes required by the Smolyak formula only grows logarithmically with  $d$ .

Different sparse grid interpolations can be constructed based on the choice of one-dimensional interpolation (3.16). One popular choice is Clenshaw–Curtis interpolation, which utilizes the Lagrange polynomial basis defined on the extrema of the Chebyshev polynomials. For any choice of  $m_i$ ,  $1 \leq i \leq d$ , these nodes are given by

$$X_i^j = -\cos \frac{\pi(j-1)}{m_i-1}, \quad j = 1, \dots, m_i, \tag{3.19}$$

To ensure the nodal sets are nested, we choose

$$m_1 = 1 \quad \text{and} \quad m_i = 2^{i-1} + 1, \quad \text{for } i > 1$$

There have been extensive studies on the approximation properties of sparse grids, particularly those based on Clenshaw–Curtis abscissas. Here, we cite one of the early results from [3]. For functions in space

$$F_d^\ell = \{f : [-1, 1]^d \rightarrow \mathbb{R} \mid \partial^{\alpha} f \text{ continuous, } \alpha_j \leq \ell, \forall j\},$$

with norm

$$\|f\| = \max\{\|D^\alpha f\|_\infty, \alpha \in \mathbb{N}_0^d, \alpha_i \leq \ell\},$$

the interpolation error follows

$$\|I - \mathcal{U}_N\| \leq C_{d,\ell} m^{-\ell} (\log m)^{(\ell+2)(d-1)+1}, \tag{3.20}$$

where  $m$  is the total number of nodes required by the sparse grid interpolation  $H_{N,d}$ . (Note there is in general no explicit formula for  $m$ .)

When quantifying aleatory uncertainty the Clenshaw–Curtis sparse grids are only appropriate when the underlying random variables possess uniform distributions. However when quantifying epistemic uncertainty this requirement can be removed. The Clenshaw–Curtis grid may not be optimal for the “true” unknown distribution, however, the resulting approximation will still exhibit the required point-wise convergence, albeit at a slower rate. Subsequently Clenshaw–Curtis sparse grid interpolation, or sparse grid interpolation for that matter, is certainly not the only choice for the collocation approach. In practice, any valid interpolation approach can be employed, so long as one can establish its convergence in the point-wise sense of (3.13).

### 3.3.2. Galerkin approach

We briefly remark that (3.10) can also be solved by the Galerkin approach. In the Galerkin approach, we seek a numerical solution  $u_n(X)$  in a polynomial space such that the residual of (3.10) is orthogonal to the polynomial space. While most of the convergence of the Galerkin solution is in the weighted  $L^p$  norm on  $I_X$ , it is possible to have the solution converge point-wise uniformly, which is what we require. This usually imposes stronger smoothness conditions on the true solution  $u$ . For example, for stochastic diffusion equation with linear form random diffusivity, it was shown that the solution is analytic in term of the random inputs [1], and numerical solution converging in point-wise sense can be used for sampling non-Gaussian process [23]. Since it is not possible to discuss the convergence of the Galerkin approach without specifying the form of (3.10), we will not engage in more discussions on this.

We also remark that there exists a pseudo-spectral collocation method [25], also known as non-intrusive gPC method. Though this method is of collocation type, its convergence is usually in  $L^p$  norm, similar to Galerkin. Therefore it is not possible to discuss its  $L^\infty$  error without specifying the underlying governing equations and we will not focus on this method as well.

### 3.3.3. Piecewise smooth case

In the discussions above we have required the solution to converge in  $\infty$ -norm in the entire domain  $I_X$ . This requires sufficient *global smoothness* of  $u$ , which is rather strong in many practical problems. In fact, the discussions can be generalized to piecewise smooth function of  $u$ . That is, there exists a finite decomposition of  $I_X^k$ ,  $k = 1, \dots, m$ , such that

$$\bigcup_{k=1}^m I_X^k = I_X, \quad I_X^i \cap I_X^j = \emptyset, \quad i \neq j,$$

and in each subdomain  $I_X^k$ ,  $k = 1, \dots, m$ ,  $u(X)$  is smooth.

In this case, a suitable numerical approach in the global sense (e.g. the sparse grid interpolation) can be applied to each subdomain separately and obtain a convergent solution (in the  $\infty$ -norm)  $u_n^k(X)$  in each subdomain  $I_X^k$ . A globally convergent solution can then be constructed by “patching” the subdomain solutions together.

$$u_n(X) = \sum_{k=1}^m u_n^k(X) \mathbb{1}_{I_X^k}(X), \tag{3.21}$$

where  $\mathbb{1}_A(s) = 1$  if  $s \in A$ ;  $\mathbb{1}_A(s) = 0$  otherwise, is the indicator function. It is easy to see that this solution will converge to  $u$  in the entire domain of  $I_X$  in the  $\infty$ -norm. Note that due to the nature of the problem (3.10), there is no continuity requirement of the solution across the subdomain interfaces. Therefore, at least on the conceptual level solving the subdomain problem is straightforward. From the practical point of view, the multi-element, or piecewise, approximation techniques developed for aleatory uncertainty can be borrowed. These include the work of [2,7,14,15,22]. Hereafter we will restrict ourselves to globally smooth problems to emphasize the new conceptual ideas related to epistemic uncertainty quantification.

### 3.4. Epistemic uncertainty analysis

When  $u_n(X)$ , the polynomial approximation of the true solution  $u(X)$ , is obtained for (3.10) and converges in the  $\infty$ -norm (3.13), it can serve as an accurate and point-wise model. We can then apply various operations on  $u_n$  instead of  $u$ . Note the operations on  $u_n$  do not require us to solve the governing equations anymore—they can be treated as post-processing steps.

Assuming information about the distribution of the random inputs  $Z$  is known *a posteriori*, then we can evaluate the solution statistics by using the  $u_n$ . This can be achieved by evaluating the statistics of  $u_n$  using the probability of  $Z$  in the domain  $I^\rho$  defined in (3.7). Let  $\rho_Z(s) = dF_Z(s)$ ,  $s \in I_Z$ , be the probability density function of the epistemic uncertain input  $Z$ , which was not known prior to the computations but is now known after the computations. Then, for example, the mean of the true solution  $v(Z)$ ,

$$\mu \triangleq \mathbb{E}[(v)(Z)] = \int_{I_Z} v(s)\rho_Z(s)ds, \tag{3.22}$$

can be approximated by

$$\mu_n \triangleq \int_{I^\rho} u_n(s)\rho_Z(s)ds. \tag{3.23}$$

The following result can be established

**Theorem 3.1.** Assume the solution of (2.1),  $v(Z)$ , is bounded and let  $C_v = \|v\|_{L^\infty(I_Z)}$ . Let  $u_n(X)$  be an approximation to the solution  $u(X)$  of (3.10) and converge in the form of (3.13) and denote

$$\epsilon_n = \|u_n(X) - u(X)\|_{L^\infty(I_X)}. \tag{3.24}$$

Then the mean of  $v$  in (3.22) and the mean of  $u_n$  in (3.23) satisfy

$$|\mu - \mu_n| \leq \epsilon_n + C_v \delta. \tag{3.25}$$

**Proof.** We first extend the domain of definition of  $v$ ,  $\rho$ , and  $u_n$  to  $I^+$ , following the definitions of the domains in (3.7), and define

$$\rho^+(s) = \mathbb{1}_{I_Z}(s)\rho_Z(s), \quad v^+(s) = \mathbb{1}_{I_Z}(s)v(s), \quad s \in I^+,$$

and

$$u_n^+(s) = \mathbb{1}_{I_X}(s)u_n(s), \quad s \in I^+.$$

Naturally,  $\rho^+$  is a probability density function on  $I^+$ . Then (3.22) can be expressed as

$$\mu = \int_{I_Z} v(s)\rho_Z(s)ds = \int_{I^+} v^+(s)\rho^+(s)ds,$$

which can be split into two parts

$$\mu = \int_{I^\rho} v^+(s)\rho^+(s)ds + \int_{I^-} v^+(s)\rho^+(s)ds = \int_{I^\rho} v(s)\rho_Z(s)ds + \int_{I^-} v^+(s)\rho^+(s)ds. \tag{3.26}$$

By using (3.23), we have

$$\mu - \mu_n = \int_{I^\rho} (v(s) - u_n(s))\rho_Z(s)ds + \int_{I^-} v(s)\rho^+(s)ds = \int_{I^\rho} (u(s) - u_n(s))\rho_Z(s)ds + \int_{I^- \cap I_Z} v(s)\rho_Z(s)ds, \tag{3.27}$$

where the property (3.11) has been used. Utilizing the condition (3.9), the main result (3.25) is established.  $\square$

The second term in (3.27),  $C_{\nu}\delta$ , is a result of truncating the “tails” of the true probability distribution of  $Z$  by using a bounded hypercube  $I_X$  to encapsulate a possibly unbounded domain  $I_Z$ . For unbounded domains, for which  $I^- \cap I_Z \neq \emptyset$ , the term  $C_{\nu}\delta$  can be made arbitrarily small by choosing a sufficiently big hypercube for  $I_X$ . If  $Z$  is in a bounded domain and the domain  $I_X$  can completely encapsulate  $I_Z$  then the term  $C_{\nu}\delta$  disappears. In this case, the error in the mean would converge to zero as long as  $u_n$  converges in the form of (3.13).

We remark that the encapsulation problem can also be used to obtain upper and lower bounds on the model observables. Consequently solving the encapsulation problem can be used as an alternative to techniques such as interval analysis [17]. The accuracy of these estimates is beyond the scope of this paper and is left for future work.

### 3.5. Mixed aleatory and epistemic uncertainty analysis

In practice, situations may arise for which the distributions of some of the random variables characterizing the input are known and some are not. The encapsulation methodology proposed here can easily be extended to such cases possessing mixed aleatory and epistemic uncertainty. Let us consider stochastic differential equations with the following form

$$\begin{cases} v_t(x, t, Y, Z) = \mathcal{L}(v), & D \times (0, T] \times I_Y \times I_Z, \\ \mathcal{B}(v) = 0, & \partial D \times [0, T] \times I_Y \times I_Z, \\ v = v_0, & D \times \{t = 0\} \times I_Y \times I_Z, \end{cases} \quad (3.28)$$

where  $Y$  is a set of random variables with known probability distribution  $F_Y(y) = P(Y \leq y)$ ,  $y \in I_Y \subseteq \mathbb{R}^r$ ,  $r \geq 1$ , and  $Z \in \mathbb{R}^s$  are a set of random variables with unknown distribution.

As in the purely epistemic case we first begin by defining and solving an encapsulation problem. With this aim we again define the encapsulation set  $I_X$  according to (3.6) which encapsulates  $I_Z$ , the “true” and unknown support of  $Z$ , with probability at least  $1 - \delta$ . The encapsulation problem is then

$$\begin{cases} u_t(x, t, Y, X) = \mathcal{L}(u), & D \times (0, T] \times I_Y \times I_X, \\ \mathcal{B}(u) = 0, & \partial D \times [0, T] \times I_Y \times I_X, \\ u = u_0, & D \times \{t = 0\} \times I_Y \times I_X. \end{cases} \quad (3.29)$$

Unlike in the purely epistemic case, the encapsulation problem is now defined in terms of the epistemic and aleatory variables. This encapsulation problem can be solved in two ways depending on whether one wants to solve the epistemic and aleatory problems separately or simultaneously:

- *Separate construction:* Different methods can be employed to quantify the epistemic  $u(\cdot, X)$  and aleatory uncertainty  $u(\cdot, Y)$ . Let  $\hat{u}_m(X)$  be an approximation to  $u(\cdot, X)$  after fixing all variables other than  $X$  and  $\tilde{u}_k(Y)$  be an approximation to  $u(\cdot, Y)$ , where the indices  $m$  and  $k$  denoting the level of approximations. Then  $u(X, Y)$  can be approximated by a tensor product of  $\hat{u}_m(X)$  and  $\tilde{u}_k(Y)$ . That is,

$$u_n(X, Y) = \hat{u}_m(X) \otimes \tilde{u}_k(Y),$$

where the index  $n$  depends on  $m$  and  $k$ . (In the case of polynomial approximation,  $n$  can be either the highest polynomial order in  $\hat{u}_m$  and  $\tilde{u}_k$  or the total order of the mixed polynomials of  $\hat{u}_m$  and  $\tilde{u}_k$ .) The construction allows us to use different methods for  $X$  and  $Y$ . For example, we can mix an accurate collocation solution  $\hat{u}_m(X)$  converging in  $L^\infty$  norm in the epistemic variable  $X$  with an accurate stochastic Galerkin solution  $\tilde{u}_k(Y)$  converging in  $L^2_{\rho_Y}$  norm in the aleatory variable  $Y$ .

- *Simultaneous construction:* Instead of treating the epistemic and aleatory variables separately, we can consider the aleatory variables as epistemic and solve the epistemic encapsulation problem (3.10), with  $I_X$  defined in such a way that it encapsulates both  $I_Z$  and  $I_Y$ . For  $r$  aleatory variables  $Y$  and  $s$  epistemic variables  $Z$ , we define

$$I_X = (\times_{i=1}^r I_{Y_i}) \times (\times_{i=1}^s I_{X_i}), \quad (3.30)$$

where  $I_{X_i}$  are bounded intervals that encapsulate  $I_{Z_i}$  with overwhelming probability. The same methods for the epistemic encapsulation problem can be used to generate an approximation in  $I_X$ . The probabilistic information associated with the aleatory variables  $Y$  can be introduced in post-processing. Additional probabilistic information for  $Z$  can be processed *a posteriori* when known. We remark that this approach requires point-wise accuracy in the entire space (3.30). This may be too strong because in general accuracy in mean square sense in the aleatory variables  $Y$  is sufficient. Point-wise accuracy is particularly hard to achieve when the aleatory variables are unbounded. In this case we may need to truncate the domain of the aleatory variables and this leads to additional “truncation” error. Therefore, the simultaneous approach is more appropriate when all the variables are bounded.

After taking into account the probability distribution of the aleatory random variables  $Y$ , the solution becomes a function of the epistemic variable  $Z$ . For example, the mean solution is

$$\mu(s) = \mathbb{E}_Y[v(Y, Z)] = \int v(y, s) dF_Y(y), \quad s \in I_Z.$$

This can be approximated by

$$\mu_n(s) = \mathbb{E}_Y[u_n(Y, X)] = \int u_n(y, s) dF_Y(y), \quad s \in I_X.$$

Note that no probability information is assigned to the variables  $X$  and  $Z$  prior to any computations.

### 4. Numerical examples

In this section, we provide several numerical tests to illustrate the implementation and convergence of the proposed methodology. In all examples, we first seek polynomial approximation to the solutions in terms of the epistemic variables. We then, in post-processing steps, assume certain probability distribution information is known *a posteriori* and then evaluate the solution statistics of the true solution and the numerical approximations and examine the accuracy of the methods. In all examples, we utilize global polynomial approximations.

#### 4.1. Ordinary differential equation

Consider

$$\frac{dv}{dt}(t) = -Z_1 v, \quad v(0) = Z_2, \tag{4.1}$$

where the parameters  $Z_1$  and  $Z_2$  are random variables representing the input uncertainty. The exact solution is

$$v(t, Z) = Z_2 \exp(-Z_1 t). \tag{4.2}$$

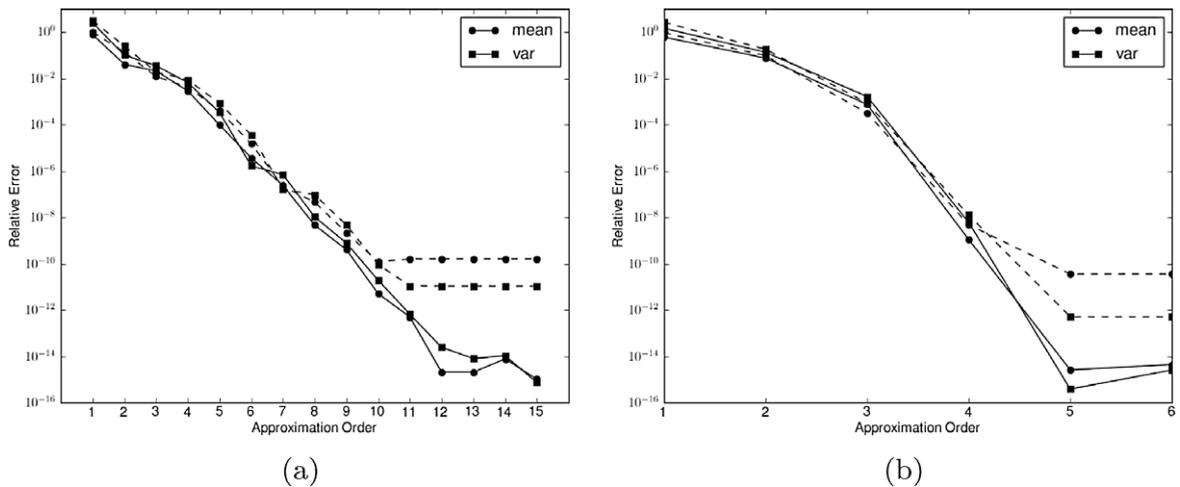
Let us assume that the distributions (and dependence) of  $Z_1$  and  $Z_2$  are unknown, except that the bounds of the parameters can be estimated with a range that is sufficiently wide.

The encapsulation problem is

$$u_t(t, X) = -X_1 u, \quad u(0) = X_2, \tag{4.3}$$

where  $X = (X_1, X_2) \in [-1, 1]^2$  after scaling.

Here, we use the Galerkin method based on Legendre polynomials to solve (4.3). This implies the numerical solution will converge in the  $L^2$  norm. However, since the solution is analytic, point-wise convergence can also be achieved. For comparison, we also present results using a sparse grid approximation of  $u$  based upon the tensor product of Lagrange polynomials defined at the Clenshaw–Curtis abscissas. Both methods provide fast converging polynomial approximations of the solution. We illustrate the convergence of the mean and variance of these approximations when the marginal and joint probability distributions are found *a posteriori* below.



**Fig. 4.1.** Convergence of the relative error in the mean and variance for the linear ODE with two dimensional ( $d = 2$ ) independent input with varying *a posteriori* distributions,  $Z_1, Z_2 \in \text{beta}(0, 1, 1, 1)$  (solid lines),  $Z_1 \in \text{beta}(0, 1, 2, 5)$  and  $Z_2 \in \text{beta}(0, 1, 1, 1)$  (dashed lines). (a) Convergence with Galerkin polynomial order. (b) Convergence with collocation sparse grid level.

4.1.1. Independent case

Let us assume the “true” (and yet unknown) distribution of  $Z$  is  $Z_1 \in \text{beta}(0, 1, \alpha_1, \beta_1), Z_2 \in \text{beta}(0, 1, \alpha_2, \beta_2)$ , where  $Z_1$  and  $Z_2$  are independent and  $\text{beta}(a, b, \alpha, \beta)$  is the beta distribution on the interval  $[a, b]$  with distribution parameters  $\alpha$  and  $\beta$ . Analytical expressions for the moments of  $v$  exist and can be used to test convergence of our numerical solutions of the encapsulation problem in  $X$ . Note in this case  $I_Z = [0, 1] \times [0, 1]$  and is completely encapsulated by  $I_X = [-1, 1]^2$ .

The moments of the numerical approximations were obtained by using multi-dimensional tensor product Gauss–Jacobi quadrature. Specifically an appropriate high-order one-dimensional quadrature rule, determined by the now known distribution of  $Z$ , was chosen for each independent variable and then a tensor product of these rules was used to construct a set of multi-dimensional quadrature nodes and associated weights. The order of the quadrature rule was chosen to match the order of the approximating polynomial. Sampling the polynomial expansion at the quadrature nodes is a post-processing process and only requires the evaluation of algebraic expressions and is thus inexpensive compared to the cost of evaluating the true model.

In Fig. 4.1 the relative error in the first two moments are shown for varying values of  $\alpha_i$  and  $\beta_i$ . Here and through out the remainder of this paper relative error is defined to be the absolute difference between the approximate and true value normalized by the true value. As the order of the Legendre–Galerkin polynomial expansion and the approximation level of the collocation sparse grid increases, the errors converge exponentially fast before reaching saturation levels.

4.1.2. Dependent case

Let us assume the “true” (and yet unknown) distribution of  $Z$  is  $Z_1 \in \text{beta}(0, 1, \alpha_1, \beta_1), Z_2$  is dependent on  $Z_1$ . Specifically let us assume that  $Z_2 = Z_1$ . This implies that  $I_Z = [0, 1]$  and can be entirely encapsulated by  $I_X = [-1, 1]^2$ . Again analytical expressions for the moments of  $v$  exist and can be used to test convergence of our numerical approximations, whose moments were obtained by selecting an appropriate high-order one-dimensional quadrature rule, determined by the now known distribution of  $Z$ , for the variables  $Z_1$ . This one-dimensional quadrature rule was then use to evaluate the moments of the approximations along the line  $Z_1 = Z_2$ .

Fig. 4.2 plots the error in the first two moments for varying values of  $\alpha_i$  and  $\beta_i$ . As the approximation level of the collocation sparse grid increases the errors converge exponentially fast before reaching saturation levels.

4.1.3. Choice of polynomial basis

In Sections 4.1.1 and 4.1.2, multi-dimensional Lagrange and Legendre polynomials were used to produce an approximation to the solution of the encapsulation problem. However any type of polynomial that satisfies (3.13) can be used.

It was shown in [28] that, in the context of aleatory uncertainty quantification, if the polynomial basis used to approximate a stochastic solution is chosen according to the distribution of the underlying random variables, better approximation accuracy can be achieved. If the optimal basis is not chosen, the rate of convergence will deteriorate. Here, we investigate the effect of the choice of the approximating polynomial on the convergence of the mean and variance of solutions subject to epistemic uncertainty.

Let us assume the “true” (and yet unknown) distributions of  $Z_i$  are independent. Fig. 4.3 shows the rate of convergence in the estimates of variance for various types of polynomial approximations of the encapsulation problem (4.3). When the optimal polynomial basis is used, estimates of the variance are obtained directly from the basis coefficients. The variance of the

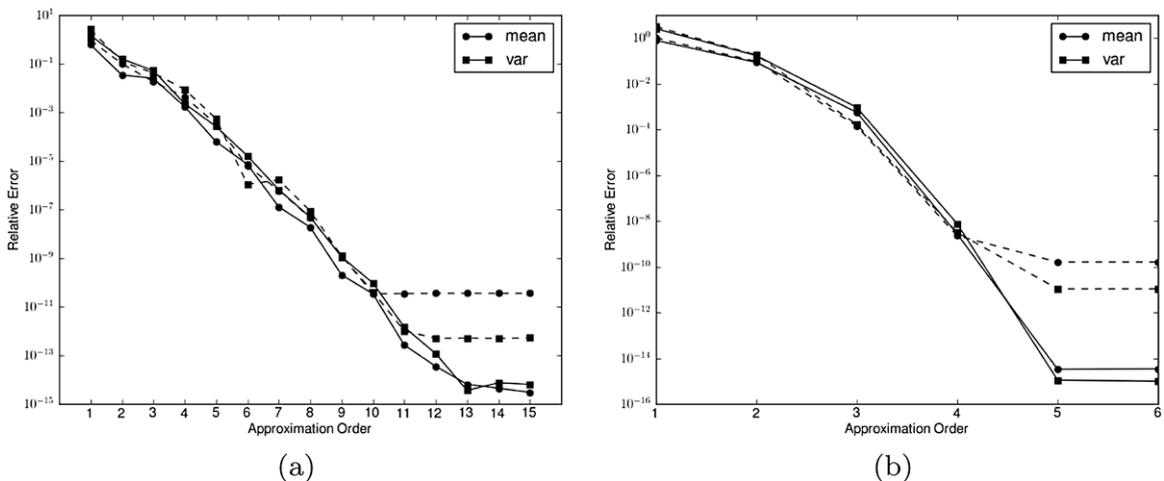
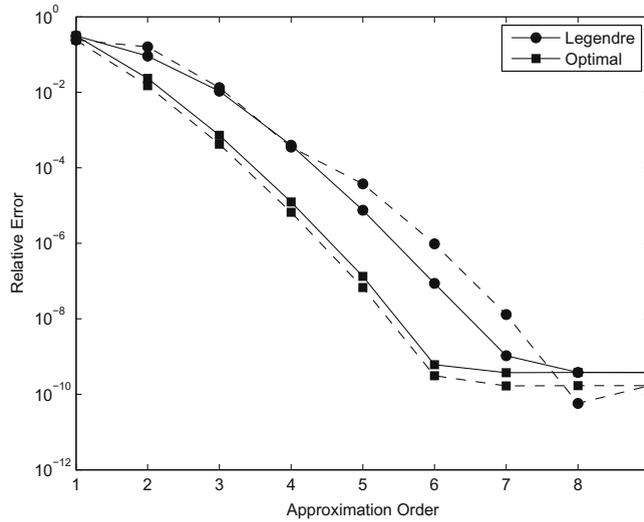


Fig. 4.2. Convergence of the relative error in the mean and variance for the linear ODE with two dimensional ( $d = 2$ ) independent input with varying  $a$  posteriori distributions,  $Z_1, \in \text{beta}(0, 1, 1, 1)$  (solid lines),  $Z_1 \in \text{beta}(0, 1, 2, 5)$  (dashed lines). In all cases  $Z_2 = Z_1$ . (a) Convergence with Galerkin polynomial order. (b) Convergence with collocation sparse grid level.



**Fig. 4.3.** Convergence of the relative error in the variance for the linear ODE with two independent input variables. Convergence is shown with respect to the order of the gpc expansion or two choices of stochastic polynomial expansions and for two different input distributions;  $Z_1, Z_2 \in \text{beta}(-1, 1, 1, 1)$  (solid lines) and  $Z_1, Z_2 \in \text{beta}(-1, 1, 2, 2)$  (dashed lines).

(non-optimal) Legendre approximation was calculated using a high-order two-dimensional tensor product Gauss–Jacobi quadrature rule.

When the type of polynomial expansion is chosen to match the distribution of the input variables, a faster of convergence is obtained than if another type was chosen. The nature of epistemic uncertainty means that an optimal basis cannot be chosen *a priori* and some accuracy penalty may have to be paid due to the lack of full probabilistic information at the time of expansion computation. If, by coincidence, the basis chosen to approximate the encapsulation problem matches the weighting functions of the underlying random variables, then the optimal convergence rate will be achieved. In most cases, however, we must select a basis that provides a reasonable compromise given the information available; e.g. if only bounds are provided and there is no justification to weight errors unequally within these bounds, then a Legendre basis is the natural choice.

#### 4.2. Random oscillator

This section investigates the performance of stochastic collocation to quantify epistemic uncertainty in a damped linear oscillator subject to external forcing with six unknown parameters. That is,

$$\frac{d^2x}{dt^2}(t, Z) + \gamma \frac{dx}{dt} + kx = f \cos(\omega t), \tag{4.4}$$

subject to the initial conditions

$$x(0) = x_0, \quad \dot{x}(0) = x_1, \tag{4.5}$$

where we assume the damping coefficient  $\gamma$ , spring constant  $k$ , forcing amplitude  $f$  and frequency  $\omega$ , and the initial conditions  $x_0$  and  $x_1$  are all uncertain, and let

$$Z = (\gamma, k, f, \omega, x_0, x_1) \in \mathbb{R}^6$$

be the epistemic variables.

The encapsulation problem is then

$$\frac{d^2x}{dt^2}(t, X) + X_1 \frac{dx}{dt} + X_2 x = X_3 \cos(X_4 t), \tag{4.6}$$

$$x(0) = X_5, \quad \dot{x}(0) = X_6, \tag{4.7}$$

where  $\mathbf{X} = (X_1, \dots, X_6) \in [-1, 1]^6$  (upon scaling) are the encapsulation variables. We employ sparse grid Lagrange interpolation at the Clenshaw–Curtis abscissas to solve the encapsulation problem.

4.2.1. Epistemic uncertainty with dependent inputs

To again illustrate the convergence of moments, let us assume the “true” (and yet unknown) distribution of  $Z$  is  $Z_i \in \text{beta}(a_i, b_i, \alpha_i, \beta_i)$ ,  $i = 1, 3, 5$  and  $Z_2$  is dependent on  $Z_1$ ,  $Z_4$  is dependent on  $Z_3$  and  $Z_6$  is dependent on  $Z_5$ . For example, let us assume  $Z_1 \in \text{beta}(0.08, 0.12, 3, 2)$  and  $Z_2 = \frac{Z_1^2}{4} + 0.01$ ,  $Z_3 \in \text{beta}(0.08, 0.12, 1, 1)$  and  $Z_4 = 10Z_3$ , and  $Z_5 \in \text{uniform}(0.45, 0.55)$  and  $Z_6 = (Z_5 - 0.5)$ .

Moments can be evaluated by collapsing the expansion in  $X$  by substitution based upon the known functional dependence and then applying a lower-dimensional quadrature rule. Here, we employed a three-dimensional quadrature rule based upon the tensor product of one-dimensional rules for  $Z_1, Z_3$  and  $Z_5$ . Values for the remaining variables were selected based upon the functional dependence specified above.

Fig. 4.4 plots the error in the first two moments at  $t = 20$ . As the order of the approximation level of the sparse grid increases the errors converge exponentially fast before reaching saturation levels.

4.2.2. Epistemic uncertainty with known covariance

In practice one may often encounter uncertainty arising from a set of random variables with normally distributed marginal distributions and known covariance. Consider  $X = (X_1, \dots, X_6) \sim N(\mathbf{0}, C)$  where the covariance matrix is a tri-diagonal matrix with non-zero entries  $\sigma_{11} = 0.03$ ,  $\sigma_{22} = 0.0009$ ,  $\sigma_{33} = 0.0003$ ,  $\sigma_{44} = 0.01$ ,  $\sigma_{55} = 0.001$ ,  $\sigma_{66} = 0.0025$ ,  $\sigma_{12} = 0.05\sigma_{11}$ ,  $\sigma_{21} = \sigma_{22}$ ,  $\sigma_{34} = 0.02\sigma_{44}$ ,  $\sigma_{43} = 0.2\sigma_{44}$ , and  $\sigma_{56} = \sigma_{65} = 0.1\sigma_{55}$ .

Unlike the previous examples the epistemic variables are now unbounded. Consequently we must construct an approximation to the encapsulation problem which captures the true input range with overwhelming probability. Here, we investigate the choice of size of the bounding hyper-region on the accuracy of the of solution moments. Fig. 4.5 plots the error in the first two moments at  $t = 20$ . As the approximation level of the collocation sparse grid increases the errors converge exponentially fast before reaching saturation levels. However, the accuracy at which saturation occurs is dependent on how “well” the input space is encapsulated. As the encapsulation probability increases, that is  $\delta$  decreases, the best possible accuracy that can be obtained by solving the encapsulation problem increases. It must be noted that the convergence rate slows with decreasing  $\delta$ , because it increases the size of the encapsulation domain. In general interpolation of a larger domain requires more evaluations of the governing equations to achieve a comparable accuracy.

The exact moments of the solution were obtained by applying high order six-dimensional Gauss–Hermite sparse grid quadrature to the governing equations. Moments of the sc approximation were obtained by applying the same quadrature rule to the numerical solution of the encapsulation problem. The Gauss–Hermite sparse grid quadrature assumes independent Gaussian variables. A Cholesky decomposition of the covariance matrix was used to generate a set of dependent realizations of  $Z$ .

4.2.3. Mixed aleatory-epistemic uncertainty

Now let us consider the uncertainty of the solution to (4.4) where the distributions of some of the variables are known and the distributions of other variables are unknown.

A simple two step iterative procedure can be used to generate such an ensemble of statistics. In this case we wish to generate an ensemble of CDFs of the solution to the governing equations at time  $t = 20$ . In the first step of each iteration a particular value of each epistemic variable is chosen from within their assumed ranges. Fixing these values we then randomly

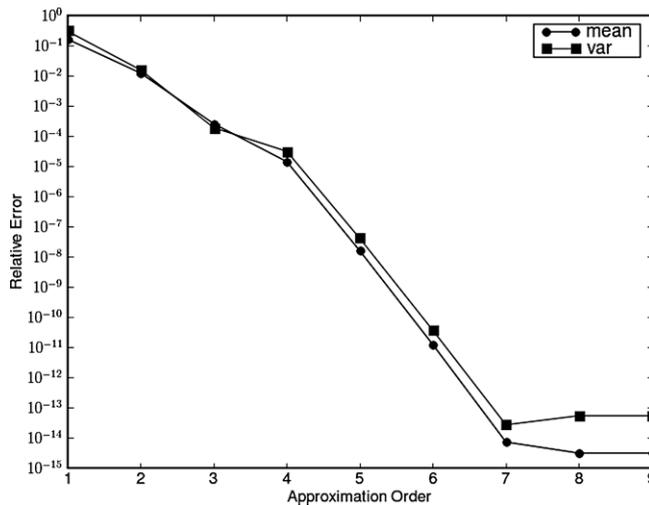


Fig. 4.4. Convergence of the relative error in the mean and variance for the damped harmonic oscillator with six dependent inputs. Convergence is shown with respect to the approximation level of the SC sparse grid.

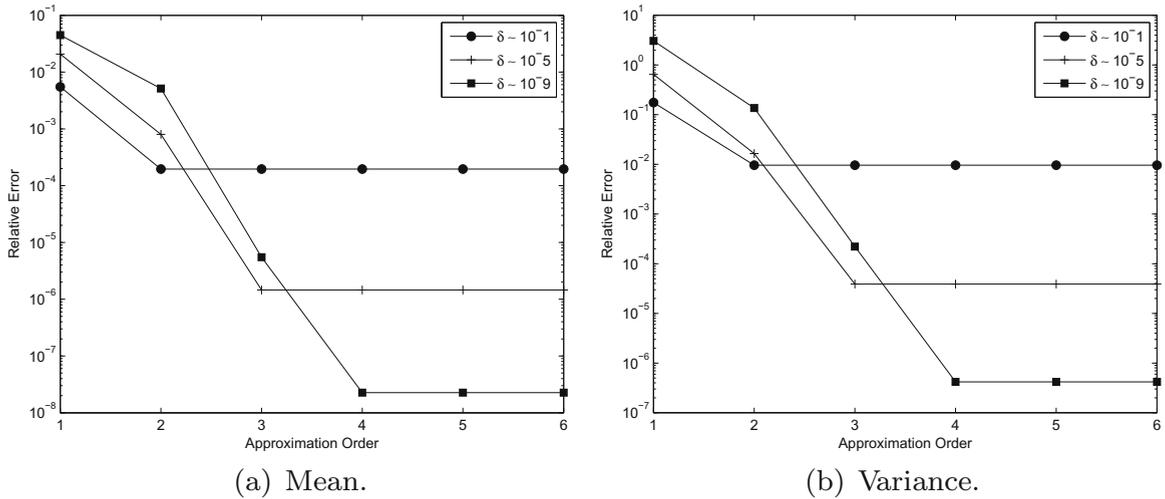


Fig. 4.5. Convergence of the relative error in the mean and variance for the damped harmonic oscillator with six dependent inputs with known covariance. Convergence is with respect to the order of the collocation sparse grid and the truncation probability  $\delta$ .

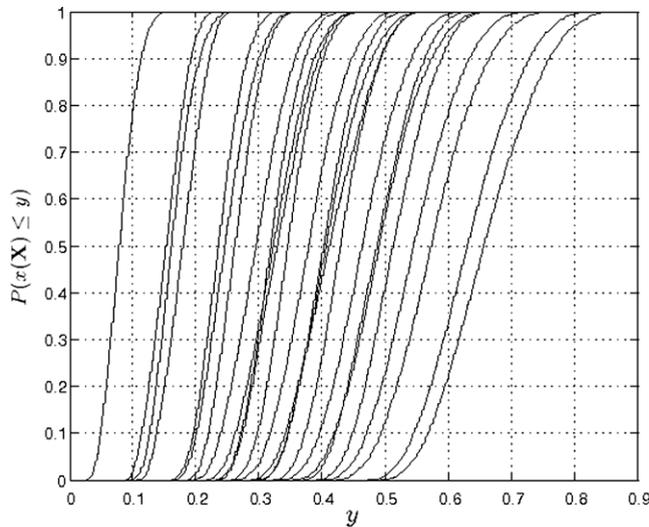


Fig. 4.6. An ensemble of 25 CDFs of the solution to the damped harmonic oscillator subject to mixed aleatory and epistemic uncertainty. Each CDF corresponds to one particular set of epistemic variables values.

sample from the aleatory variables in a standard probabilistic manner. These samples are then used to evaluate the polynomial approximation of the encapsulation problem. Following this heuristic, each set of epistemic variables generates a full distributional description and corresponding statistical metrics, such as moments, for the output quantities.

Let the variables  $Z_1, Z_2, Z_3$ , and  $Z_5$  have known distributions with  $Z_1 \sim \text{beta}(0, 1, 0, 0)$ ,  $Z_2 = \frac{Z_1^2}{4} + 0.01$ ,  $Z_3 \sim \text{beta}(0, 1, 1, 1)$  and  $Z_5 \sim \text{beta}(0, 1, 2, 1)$  and let the two remaining input variables  $Z_4$  and  $Z_6$  be epistemic variables that lie within the following ranges:  $Z_4 \in [0.8, 1.2]$  and  $Z_6 \in [-0.05, 0.05]$ . Now let us construct a sparse grid collocation approximation to the encapsulation problem using the simultaneous construction outlined in Section 3.5.

Fig. 4.6 plots an ensemble of CDFs of the numerical solution to (4.4) for 25 realizations of the two epistemic variables. Each epistemic variable was assumed to take five discrete values  $Z_i^k$  equally spaced throughout their corresponding ranges  $[a_i, b_i]$ ,  $i = 4, 6$ . Specifically we choose  $Z_i^k = a_i + k(b_i - a_i)/4$ ,  $k = 0, \dots, 4$ . For each of the 25 combinations of  $Z_i^k$ , Monte-Carlo sampling of the aleatory variables is used to generate a CDF from evaluation of the polynomial approximation. It is evident that the two epistemic variables have a large influence on the distribution of the output. This could indicate that effort should be focused on more accurately reducing the range of these variables.

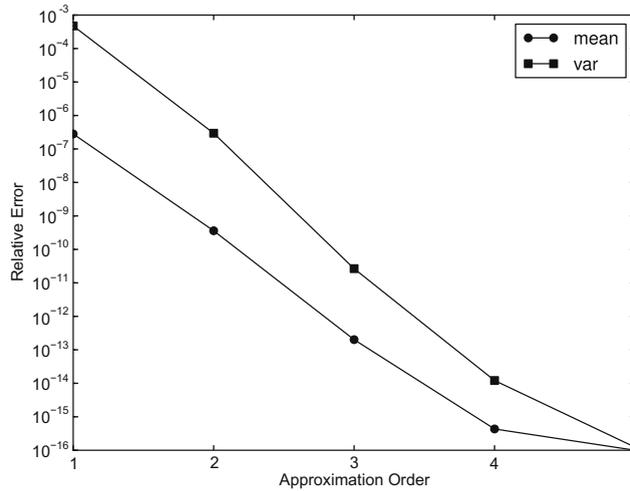


Fig. 4.7. Convergence of the relative error in the mean and variance for the homogeneous diffusion equation with six dependent inputs. Convergence is with respect to the order of the gpc expansion, at the spatial location  $x = 0.848925247397$ .

### 4.3. Homogeneous diffusion equation

In this section, we consider the homogeneous diffusion equation in one-spatial dimension subject to epistemic uncertainty in the diffusivity coefficient. Attention is restricted to the one-dimensional physical space to avoid unnecessary complexity. The procedure described here can easily be extended to higher physical dimensions. Consider the following problem with  $d \geq 1$  random dimensions:

$$\frac{d}{dx} \left[ a(x, Z) \frac{du}{dx}(x, Z) \right] = 0, \quad (x, Z) \in (0, 1) \times I_Z \tag{4.8}$$

subject to the physical boundary conditions

$$u(0) = 0, \quad u(1) = 0. \tag{4.9}$$

Furthermore assume that the random diffusivity satisfies

$$a(x, Z) = 1 + \sigma \sum_{k=1}^d \frac{1}{k^2 \pi^2} \cos(2\pi k x) Z_k, \tag{4.10}$$

where  $Z_k \in [-1, 1]$ ,  $k = 1, \dots, d$  are independent and uniformly distributed random variables. The form of (4.10) is similar to that obtained from a Karhunen–Loève expansion and satisfies the auxiliary properties

$$\mathbb{E}[a(x, Z)] = 1 \quad \text{and} \quad 1 - \frac{\sigma}{6} < a(x, Z) < 1 + \frac{\sigma}{6}. \tag{4.11}$$

This is the same test case used in [27].

Again we construct an appropriate encapsulation problem and solve it using the Legendre–Galerkin method. Specifically, we employ the efficient spectral Galerkin iterative solver discussed in [29]. A high spatial resolution is used to ensure that the associated errors can be neglected in the following analysis.

Whereas previous discussions have focused on singular parameter dependence, here we investigate the performance of the proposed method for multi-parameter dependence. Let us assume the “true” (and yet unknown) distribution of  $Z$  is  $Z_1 \in \text{beta}(0, 1, 3, 2)$ , and  $Z_3 \in \text{beta}(-1, 0, 1, 1)$  and  $Z_5 \in \text{beta}(-0.5, 0.5, 0, 0)$ ,  $Z_2 = Z_1 Z_5$ ,  $Z_4 = (Z_1^2 + 1) Z_3$ , and  $Z_6 = -Z_5$  and  $\sigma = 4$ . The convergence of the mean and variance of the encapsulation problem at  $x = 0.848925247397$  are shown in Fig. 4.7. Despite the non-linear dependence between the random variables the fast rate of convergence is still maintained. No analytical solution is available so convergence is analyzed against a high order Legendre–Galerkin approximation of the solution.

## 5. Conclusions

In this paper, we proposed a framework for quantifying epistemic uncertainty. The methodology presented is a generalization of traditional aleatory uncertainty quantification that allows one to seamlessly switch between epistemic, aleatory

and mixed epistemic–aleatory uncertainty analysis. The validity and effectiveness of our approaches is illustrated through several examples.

The approach is based on solution of an “encapsulation problem” which generates a solution to the governing equations in a domain that encloses the true probability space with overwhelming probability. No distributional information about any of the variables needs be assumed, only estimates of the ranges of the variables are needed. Once the bounds have been specified, a polynomial approximation can be constructed in the encapsulation domain. The polynomial approximation to the encapsulation problem is chosen to converge point-wise throughout the input space, thus it is also accurate on a subset of this space. As long as this point-wise convergence is obtained, the polynomial solution of the encapsulation problem can be used as an effective model for the true solution on the true domain.

Once the polynomial approximation within the encapsulation domain has been computed, it can be employed within epistemic analyses such as interval analysis or evidence theory, within sensitivity analysis studies to explore the importance of epistemic parameters and allocate experimental resources, and ultimately within *a posteriori* aleatory analyses following collection of additional experimental data. In this paper, we focus on the *a posteriori* evaluation of solution statistics and demonstrate convergence of statistics following the introduction of additional information on functional dependence or correlation, distributional form, or both.

The encapsulation approach can readily handle dependencies between input variables. If the functional dependence becomes known *a posteriori*, then the relationships can be used to collapse the dimensionality of the polynomial approximation and quadrature methods can then be applied on this lower-dimensional space to obtain estimates of moments. We show that exponential convergence can be obtained for correlated normals by utilizing a Cholesky decomposition to map a set of independent variables (needed to construct the polynomial approximation) to a set of dependent variables. Although not presented, such a procedure could be extended to correlated non-normals provided a variable transformation exists, for example the Nataf transformation.

If the distributional form of the epistemic variables becomes known *a posteriori*, then solution statistics can be evaluated as a post-processing step. While the polynomial basis selected *a priori* will not in general be optimal for this *a posteriori* post-processing, this suboptimal weighting of polynomial approximation errors is an algorithmic cost that must be paid for having imperfect characterization of uncertainties at the time of approximation construction. The modeler can minimize this penalty by tailoring the basis to the available information to the extent possible, but in the case of a pure interval-based epistemic uncertainty description, there is no justification to weight errors unequally within the interval and a Legendre basis is the logical choice. It is demonstrated that exponentially-fast convergence rates can nonetheless be obtained for the *a posteriori* solution statistics despite the lack of complete information at expansion construction time.

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