

Uncertainty Quantification for Polynomial Systems via Bernstein Expansions

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This paper presents a unifying framework to uncertainty quantification for systems having polynomial response metrics that depend on both aleatory and epistemic uncertainties. The approach proposed, which is based on the Bernstein expansions of polynomials, enables bounding the range of moments and failure probabilities of response metrics as well as finding supersets of the extreme epistemic realizations where the limits of such ranges occur. These bounds and supersets, whose analytical structure renders them free of approximation error, can be made arbitrarily tight with additional computational effort. Furthermore, this framework enables determining the importance of particular uncertain parameters according to the extent to which they affect the first two moments of response metrics and failure probabilities. This analysis enables determining the parameters that should be considered uncertain as well as those that can be assumed to be constants without incurring significant error. The analytical nature of the approach eliminates the numerical error that characterizes the sampling-based techniques commonly used to propagate aleatory uncertainties as well as the possibility of under predicting the range of the statistic of interest that may result from searching for the best- and worst-case epistemic values via nonlinear optimization or sampling.

I. Introduction

Uncertainty Quantification (UQ) is the process of determining the effect of input uncertainties on response metrics of interest. Denote by \mathbf{p} the input parameter vector whose value

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is subject to uncertainty. These uncertainties may be classified as either *aleatory*, which are parameters subject to inherent and irreducible variability, or *epistemic*, which are reducible uncertainties resulting from a lack of knowledge. While the value assumed by aleatory variables is expected to change for a given set of operating conditions (e.g., mass of fuel within a rocket), epistemic variables are unknown constants (e.g., mass of a structure).

This paper studies the performance and reliability of a system whose response metrics are polynomial functions of the uncertain parameters. Regarding performance, the acceptability of the system depends upon the most likely outcome of a response metric. The performance analysis of a system consists of evaluating low order moments of the performance function for a given probabilistic model of the uncertainty. Regarding reliability, the acceptability of the system depends upon its ability to satisfy several design requirements simultaneously. These requirements, which are represented by a set of inequality constraints, depend on \mathbf{p} . The system is deemed acceptable if all constraints are satisfied. The reliability analysis of a system consists of evaluating the probability of violating at least one of the requirements.

A common approach to quantifying the effects of both aleatory and epistemic uncertainties is to perform nested sampling. This involves drawing samples of the epistemic variables in an outer loop and performing an UQ for the aleatory variables in an inner loop. In this fashion, ensembles of cumulative distribution functions, where each distribution represents the uncertainty generated by sampling over the aleatory variables, are generated. Nested iteration tends to be computationally expensive. Consequently, the nested sampling must often be under-resolved, particularly at the epistemic outer loop, resulting in an under-prediction of ranges of values of the response metric. Methods for propagating epistemic uncertainties, including interval-value probability,² second order probability,³ imprecise probability theory and Dempster-Shafer theory of evidence,¹⁰ suffer from such deficiencies. Methods that replace the outer sampling loop with an optimization loop have been proposed in [1]. Even though these methods are more efficient than sampling-based methods, their inability to guarantee convergence to the global optima may also result in under-estimates of the ranges of the statistics of interest.

A key feature of this contribution is that the distinction between aleatory and epistemic variables implied by their definition is made consistently both qualitatively and quantitatively. While aleatory uncertainties are manipulated according to long-standing concepts of probability theory, epistemic uncertainties are manipulated using properties of the Bernstein expansion of polynomials. In the proposed context each response metric becomes a random process. This family of random variables is parameterized by the value of the epistemic variables. In regard to the management of aleatory uncertainties, the framework proposed enables bounding tightly and rigorously the value of statistics supporting conventional UQ analyses (e.g. tight, formally verifiable ranges containing the failure probability range are calculated). In regard to the management of epistemic variables, the framework proposed enables bounding tightly and rigorously the epistemic realizations leading to the extreme values of such statistics (e.g., the realization of the epistemic variable leading to the largest failure probability). These bounds can be made arbitrarily small with additional computational effort.

The strategies proposed yield exact results: the computed bound of a extreme statistic does not suffer from numerical or approximation error while the convergence to the critical epistemic point realizing this extreme value is guaranteed. While standard probabilistic methods, such as polynomial chaos, Monte Carlo sampling, interval analysis, imprecise

probabilities, FORM, etc., cannot bound the approximation error present in their estimate of statistics, the identification of the extreme values attained by such statistics is out of their scope. As compared to methods based on interval analysis [5], whose results are also formally verifiable, the bounds proposed are better since they can always be made to converge to the set being bounded, e.g. bounds based on interval arithmetic suffer from irreducible conservatism when the requirement functions have repeated uncertain parameters. As compared to methods where the search for critical epistemic values is carried out using nonlinear programming or sampling, the proposed strategy eliminates the possibility of under-predicting the range of the statistic of interest, i.e., the search for the extrema of non-convex functions via nonlinear optimization may converge to non-global optima, thereby producing a UQ assessment that under-predicts the actual range. Furthermore, this framework enables the consideration of uncertainty models comprised of arbitrarily and possibly dependent aleatory variables, the substantial desensitization of the calculations from the assumed uncertainty model as well as the accommodation for changes in such a model with a small amount of computational effort. On the down side, as with all the UQ methods listed above, “the curse of dimensionality” restricts the applicability of the proposed strategies to systems with a moderate number of uncertainties.

This paper is organized as follows. Basic concepts and notions are introduced in Sections II and III. Section IV presents strategies for UQ in the presence of aleatory uncertainties. This is followed by Section V where developments for UQ in the presence of epistemic and aleatory uncertainties are made. Low-dimensional, easily reproducible examples are used to benchmark the scope of framework. Finally, a few concluding remarks close the paper.

II. Basic Concepts and Notions

In a system that depends on the uncertain parameter \mathbf{p} , response metrics are real-valued functions defined on a *master domain* $\mathcal{D} \subseteq \mathbb{R}^s$. These metrics include performance functions and requirements functions. A performance function, such as cost, is a metric used to evaluate a system’s performance. A reliability requirement is an admissible range of variation for a performance function, e.g., cost not exceeding the available budget. The functions prescribing reliability requirements will be called requirements functions. While a performance function will be denoted by $g(\mathbf{p})$, where $g : \mathcal{D} \rightarrow \mathbb{R}$, the reliability requirements are prescribed as the vector inequality^a $\mathbf{g}(\mathbf{p}) < \mathbf{0}$, where $\mathbf{g} : \mathcal{D} \rightarrow \mathbb{R}^v$.

The *failure domain*, denoted as $\mathcal{F} \subset \mathbb{R}^s$, is comprised of the uncertain parameter realizations that fail to satisfy at least one of the requirements. Specifically, the failure domain is given by

$$\mathcal{F} = \bigcup_{i=1}^s \{\mathbf{p} : \mathbf{g}_i(\mathbf{p}) \geq 0\} = \{\mathbf{p} : w(\mathbf{p}) \geq 0\}, \quad (1)$$

where $w(\mathbf{p}) = \max_{i \leq v} \{\mathbf{g}_i(\mathbf{p})\}$ is the *worst-case requirement function*. The *safe domain*, given by $\mathcal{S} = C(\mathcal{F})$, where $C(\cdot)$ denotes the *complement set operator* given by $C(\mathcal{Z}) = \mathcal{D} \setminus \mathcal{Z}$, consists of the parameter realizations satisfying all the design requirements.

^aThroughout this paper, it is assumed that vector inequalities hold component-wise, super-indices denote a particular vector or set, and sub-indices refer to vector components; e.g., $\mathbf{p}_i^{(j)}$ is the i th component of the vector $\mathbf{p}^{(j)}$.

Techniques for bounding \mathcal{F} and \mathcal{S} will be presented below. The resulting bounding sets are comprised of hyper-rectangles. The *hyper-rectangle* $\mathcal{R} \in \mathbb{R}^s$, whose “lower left” and “upper right” corners are at \mathbf{x} and \mathbf{y} , with $\mathbf{x} < \mathbf{y}$, is given by

$$\mathcal{R}(\mathbf{x}, \mathbf{y}) = \{\mathbf{p} : \mathbf{x} < \mathbf{p} \leq \mathbf{y}\} = (\mathbf{x}_1, \mathbf{y}_1] \times (\mathbf{x}_2, \mathbf{y}_2] \times \cdots \times (\mathbf{x}_s, \mathbf{y}_s], \quad (2)$$

where the latter expression is the Cartesian product of intervals which exclude the left endpoint and include the right. Hyper-rectangles defined this way can be sub-divided into smaller hyper-rectangles without overlap, so that each point of the original hyper-rectangle falls into exactly one of the sub-dividing hyper-rectangles. Under these conditions, the larger hyper-rectangle is said to have been *partitioned* or *subdivided* into smaller hyper-rectangles. If $\rho(\mathcal{R}) = \{\mathcal{R}_1, \dots, \mathcal{R}_t\}$ is a pairwise disjoint collection of hyper-rectangles where $\mathcal{R} = \mathcal{R}_1 \cup \dots \cup \mathcal{R}_j$, then ρ is a partition of \mathcal{R} . A bisection-based subdivision of $\mathcal{R} \subset \mathbb{R}^s$ in the i th direction, $i \leq s$, is given by

$$\rho(\mathcal{R}(\mathbf{x}, \mathbf{y})) = \{\mathcal{R}(\mathbf{x}, \mathbf{x} + \mathbf{w}), \mathcal{R}(\mathbf{y} - \mathbf{w}, \mathbf{y})\}, \quad (3)$$

where $\mathbf{w} = [\mathbf{y}_1 - \mathbf{x}_1, \dots, (\mathbf{y}_i - \mathbf{x}_i)/2, \dots, \mathbf{y}_s - \mathbf{x}_s]$.

The uncertainties considered in this paper are classified as either epistemic or aleatory. Denote by $\mathbf{e} \in \mathbb{R}^e$ a subvector of \mathbf{p} containing the epistemic variables, and by $\mathbf{a} \in \mathbb{R}^a$ a subvector of \mathbf{p} containing the aleatory variables, such that $a + e = s$. We will use non-probabilistic uncertainty models for \mathbf{e} and probabilistic ones for \mathbf{a} . Epistemic variables will be modeled by a bounded set. This set, called the *support set*, will be denoted as $\Delta_e \subseteq \mathbb{R}^e$. Each epistemic variable is modeled by providing an interval within which its value lies. Therefore, Δ_e is the Cartesian product of these intervals. A probabilistic uncertainty model on the other hand, prescribes a measure of probability to each member of a set. Aleatory parameters will be modeled as random variables. This model is fully prescribed by the joint Probability Density Function (PDF) $f(\mathbf{a}) : \Delta_a \subseteq \mathbb{R}^a \rightarrow \mathbb{R}$, or equivalently, by the Cumulative Distribution Functions (CDF) $F(\mathbf{a}) : \Delta_a \subseteq \mathbb{R}^a \rightarrow [0, 1]$. Note that $\Delta_a \times \Delta_e \subseteq \mathcal{D}_a \times \mathcal{D}_e = \mathcal{D}$. Not requiring the support set to fill up the master domain provides the freedom to change the uncertainty model without having to repeat calculations.

The failure domain can also be described as

$$\mathcal{F} = \bigcup_{\mathbf{e} \in \Delta_e} \mathcal{F}_a(\mathbf{e}), \quad (4)$$

where

$$\mathcal{F}_a(\mathbf{e}) \triangleq \{\mathbf{p} = \langle \mathbf{a}, \mathbf{e} \rangle : \mathbf{g}(\mathbf{p}) > \mathbf{0}\}, \quad (5)$$

is a set value function of the epistemic uncertainty.

The mean, variance and failure probability associated with the uncertainty model of the aleatory variables are

$$E[g(\mathbf{p})] = \int_{\Delta_a} g(\mathbf{p}) f(\mathbf{a}) d\mathbf{a}, \quad (6)$$

$$V[g(\mathbf{p})] = E[g^2(\mathbf{p})] - E[g(\mathbf{p})]^2, \quad (7)$$

$$P[\mathcal{F}] = \int_{\mathcal{F}_a} f(\mathbf{a}) d\mathbf{a}, \quad (8)$$

where $E[\cdot]$, $V[\cdot]$ and $P[\cdot]$ are the mean, variance and probability operators on the probability space Δ_a . When some of the uncertain parameters are epistemic variables, these statistics become random processes parameterized by \mathbf{e} . When all uncertain parameters are aleatory, these statistics are constants. The subscript “ a ” in \mathcal{F}_a and Δ_a will be omitted hereafter since its meaning can be inferred from context.

III. Bernstein Expansion

The image of a hyper-rectangle when mapped by a multivariable polynomial is a bounded interval. By expanding that polynomial using a Bernstein basis over the rectangle, rigorous bounds to such an interval can be calculated by mere algebraic manipulations. Bernstein polynomials^{6,11} will be used for determining if a hyper-rectangle \mathcal{R} is fully contained in the failure/safe domain or not. The outcome of the set containment test presented below depends exclusively on how much refinement of \mathcal{R} the analyst is willing to perform. The refinement of \mathcal{R} is determined by the number and size of subrectangles in a partition of \mathcal{R} . Better refinements can always be used to render the set containment tests conclusive. The mathematical foundation of this approach is presented next.

The Bernstein expansion first requires mapping \mathcal{R} into the unit hyper cube. Let $\mathcal{R} \subseteq \mathcal{D}$ be an arbitrary hyper-rectangle in the master domain. Denote by $\mathbf{u} = U(\mathbf{p})$ an affine transformation that maps the hyper-rectangle \mathcal{R} onto the unit hyper-cube $\mathcal{U} = \mathcal{R}(\mathbf{0}, \mathbf{1})$. Let g be an arbitrary polynomial in \mathbb{R}^s . Then $f(\mathbf{u}) = g(U^{-1}(\mathbf{u}))$ is a polynomial in \mathcal{U} . Note that the extrema of g on \mathcal{R} are identical to the extrema of f in \mathcal{U} .

For simplicity in the presentation we first consider a univariate polynomial. Since \mathbf{p} , \mathbf{u} and \mathbf{g} are scalars here, we will represent them as p , u and g without the bold font. The transformation of g into the unit cube leads to

$$f(u) = \sum_{i=0}^n a_i u^i, \quad (9)$$

whose Bernstein expansion is given by

$$f(u) = \sum_{i=0}^n b_i(\mathcal{R}, g) B_i^n(u), \quad (10)$$

where

$$B_i^n(u) = \binom{n}{i} u^i (1-u)^{n-i}, \quad (11)$$

is the i th Bernstein polynomial of degree n (i.e., an element of the basis) and

$$b_i(\mathcal{R}, g) = \sum_{j=0}^i \frac{\binom{i}{j}}{\binom{n}{j}} a_j, \quad (12)$$

is the i th Bernstein coefficient. Some fundamental properties of this basis are $\sum B_i^n(u) = 1$ (normalization), $0 \leq B_i^n(u) \leq 1$ for $0 \leq u \leq 1$ (boundedness), and $B_i^n(u) = B_{n-i}^n(1-u) > 0$ (symmetry). Some of the Bernstein coefficients assume the same value taken by the

polynomial at the vertices of a hyper-rectangle. This leads to the “free function evaluation property”, which is given by

$$f(0) = b_0(\mathcal{R}, g), \quad (13)$$

$$f(1) = b_n(\mathcal{R}, g). \quad (14)$$

The range enclosing property is described next. Suppose \mathcal{R} is a hyper-rectangle and $\{b_i(\mathcal{R}, g) : 0 \leq i \leq n\}$ are the Bernstein coefficients of g on \mathcal{R} . The range enclosing property dictates that, for $p \in \mathcal{R}$, $\min_{0 \leq i \leq n} b_i(\mathcal{R}, g) \leq g(p) \leq \max_{0 \leq i \leq n} b_i(\mathcal{R}, g)$. Tighter bounds are obtained if \mathcal{R} is subdivided. In particular, if $\rho(\mathcal{R}) = \{\mathcal{R}_1, \dots, \mathcal{R}_t\}$, we have that, for all $p \in \mathcal{R}$,

$$\underline{g}(p, \rho) \leq g(p) \leq \bar{g}(p, \rho), \quad (15)$$

where

$$\underline{g}(p, \rho) = \sum_{j=1}^t \min_{0 \leq i \leq n} \{b_i(\mathcal{R}_j, g)\} I(p; \mathcal{R}_j), \quad (16)$$

$$\bar{g}(p, \rho) = \sum_{j=1}^t \max_{0 \leq i \leq n} \{b_i(\mathcal{R}_j, g)\} I(p; \mathcal{R}_j), \quad (17)$$

where $I(\cdot; \mathcal{R}_j)$ is the *indicator function* of \mathcal{R}_j ; i.e., $I(p; \mathcal{R}_j) = 1$ if $p \in \mathcal{R}_j$, $I(p; \mathcal{R}_j) = 0$, otherwise. Each of \underline{g} and \bar{g} is constant on each set \mathcal{R}_j . We call \underline{g} and \bar{g} the *Bernstein lower and upper function bounds*, respectively, of g .

The multivariate polynomial case is considered next. Define the multi-index \mathbf{i} to be a vector of non-negative integers of length s . The monomial $\mathbf{u}_1^{i_1} \mathbf{u}_2^{i_2} \cdots \mathbf{u}_s^{i_s}$ is abbreviated as $\mathbf{u}^{\mathbf{i}}$. A s -variate polynomial can be represented as

$$f(\mathbf{u}) = \sum_{\mathbf{0} \leq \mathbf{i} \leq \mathbf{n}} a_{\mathbf{i}} \mathbf{u}^{\mathbf{i}}, \quad (18)$$

where $\mathbf{u} \in \mathcal{U}$. The Bernstein expansion of (18) is given by

$$f(\mathbf{u}) = \sum_{\mathbf{0} \leq \mathbf{i} \leq \mathbf{n}} b_{\mathbf{i}}(\mathcal{R}, g) B_{\mathbf{i}}^{\mathbf{n}}(\mathbf{u}), \quad (19)$$

where

$$B_{\mathbf{i}}^{\mathbf{n}}(\mathbf{u}) = B_{i_1}^{n_1}(\mathbf{u}_1) \cdots B_{i_s}^{n_s}(\mathbf{u}_s) \quad (20)$$

is the \mathbf{i} th Bernstein polynomial of degree \mathbf{n} and

$$b_{\mathbf{i}}(\mathcal{R}, g) = \sum_{\mathbf{j} \leq \mathbf{i}} \left(\prod_{k=1}^s \frac{\binom{i_k}{j_k}}{\binom{n_k}{j_k}} \right) a_{\mathbf{j}}, \quad (21)$$

for $\mathbf{0} \leq \mathbf{i} \leq \mathbf{n}$, is the \mathbf{i} th Bernstein coefficient. In this setting the free function evaluation property is

$$f(\langle \mathbf{i}_1/\mathbf{n}_1, \dots, \mathbf{i}_s/\mathbf{n}_s \rangle) = b_{\mathbf{i}}(\mathcal{R}, g), \quad (22)$$

where \mathbf{i} is an element of $\{0, \mathbf{n}_1\} \times \cdots \times \{0, \mathbf{n}_p\}$. The range enclosing property is as follows: suppose \mathcal{R} is a hyper-rectangle and $\{b_i(\mathcal{R}, g) : \mathbf{0} \leq \mathbf{i} \leq \mathbf{n}\}$ are the Bernstein coefficients of g on \mathcal{R} . The range enclosing property dictates that, for $\mathbf{p} \in \mathcal{R}$, $\min_{\mathbf{0} \leq \mathbf{i} \leq \mathbf{n}} b_i(\mathcal{R}, g) \leq g(\mathbf{p}) \leq \max_{\mathbf{0} \leq \mathbf{i} \leq \mathbf{n}} b_i(\mathcal{R}, g)$. As before, tighter bounds are obtained if Bernstein expansions over partitions of \mathcal{R} are calculated. Specifically,

$$\underline{g}(\mathbf{p}, \rho) \leq g(\mathbf{p}) \leq \bar{g}(\mathbf{p}, \rho), \quad (23)$$

for all $\mathbf{p} \in \mathcal{R}$ where

$$\underline{g}(\mathbf{p}, \rho) = \sum_{j=1}^t \min_{\mathbf{0} \leq \mathbf{i} \leq \mathbf{n}} \{b_i(\mathcal{R}_j, g)\} I(\mathbf{p}; \mathcal{R}_j), \quad (24)$$

$$\bar{g}(\mathbf{p}, \rho) = \sum_{j=1}^t \max_{\mathbf{0} \leq \mathbf{i} \leq \mathbf{n}} \{b_i(\mathcal{R}_j, g)\} I(\mathbf{p}; \mathcal{R}_j). \quad (25)$$

As before, \underline{g} and \bar{g} are constant on each sub-rectangle \mathcal{R}_j . If $\mathbf{p}^{(j)}$ is the center of \mathcal{R}_j , these constant values are equal to $\underline{g}(\mathbf{p}^{(j)})$ and $\bar{g}(\mathbf{p}^{(j)})$. Since g is a continuous function on a connected set, we have

$$\text{Range}(g) = \left[\min_{\mathbf{p} \in \mathcal{R}} g(\mathbf{p}), \max_{\mathbf{p} \in \mathcal{R}} g(\mathbf{p}) \right] \subseteq \left[\min_{\mathbf{p} \in \mathcal{R}} \underline{g}(\mathbf{p}), \max_{\mathbf{p} \in \mathcal{R}} \bar{g}(\mathbf{p}) \right]. \quad (26)$$

If the partition of \mathcal{R} is successively refined so that the maximum volume of the subsets approaches zero, the end points of the bounding interval converge to the global extrema of g .

A strategy for bounding the values of \mathbf{p} where the global extrema of a polynomial occur is presented next. Let ρ be a partition of \mathcal{R} and let \mathbf{p}_* and \mathbf{p}^* denote the sets of global minima and global maxima, respectively, of $g(\mathbf{p})$ over the hyper-rectangle. The lower and upper bounding functions in (24-25) can be used to calculate supersets of \mathbf{p}_* and \mathbf{p}^* . These supersets, denoted hereafter as \mathcal{P}_* and \mathcal{P}^* , are given by

$$\mathcal{P}_* = \bigcup_j \left\{ \mathcal{R}_j : \underline{g}(\mathbf{p}^{(j)}) \leq \min_{\mathbf{p} \in \mathcal{R}} \bar{g}(\mathbf{p}) \right\} \supset \mathbf{p}_*, \quad (27)$$

$$\mathcal{P}^* = \bigcup_j \left\{ \mathcal{R}_j : \bar{g}(\mathbf{p}^{(j)}) \geq \max_{\mathbf{p} \in \mathcal{R}} \underline{g}(\mathbf{p}) \right\} \supset \mathbf{p}^*. \quad (28)$$

Therefore, the superset containing the point where $g(\mathbf{p})$ attains its global minima, \mathbf{p}_* , is comprised of all rectangles where the minima of the upper bounding function \bar{g} is larger than the lower bounding function \underline{g} . Because the optimizations at the right hand side of the inequalities entail finding the extrema of piecewise constant functions over a finite partition of \mathcal{R} , they can be determined exactly in a finite number of steps^b. The supersets \mathcal{P}_* and \mathcal{P}^* approach \mathbf{p}_* and \mathbf{p}^* respectively as the partition of \mathcal{R} becomes finer. The mathematical

^bSmaller supersets \mathcal{P}_* and \mathcal{P}^* result from replacing the arguments of the min and max operators in Equations (27) and (28) with a vector comprised of all free function evaluations, i.e., Equation (22) for all the elements of the partition.

foundation supporting the polynomial bounds guarantees that \mathcal{P}_* and \mathcal{P}^* will contain all global extrema regardless of their number and their location. Equations (26) yield lower and upper bounds of the extrema of $g(\mathbf{p})$ while Equations (27) and (28) are supersets of the location of such extrema.

The preceding analysis of a single polynomial function can be applied on a component by component basis to the vector \mathbf{g} prescribing the failure domain. For a given partition of \mathcal{R} , the preceding analysis is applied to each component of \mathbf{g} to determine the bounding functions in (23). These functions can be used to calculate bounds of the worst-case requirement function in (1). The lower and upper bounding functions of w , denoted as \underline{w} and \bar{w} , are given by

$$\underline{w}(\mathbf{p}, \rho) = \sum_{j=1}^t \left(\max_{i \leq g} \underline{g}_i(\mathbf{p}^{(j)}) \right) I(\mathbf{p}, \mathcal{R}_j), \quad (29)$$

$$\bar{w}(\mathbf{p}, \rho) = \sum_{j=1}^t \left(\max_{i \leq g} \bar{g}_i(\mathbf{p}^{(j)}) \right) I(\mathbf{p}, \mathcal{R}_j), \quad (30)$$

where the indicator function I was defined earlier. As before, \underline{w} and \bar{w} are piecewise constant on each member of the partition. The following theorems, which make use of these bounding functions, enable determining whether a set $\mathcal{Q} \in \mathbb{R}^s$ is fully contained (or not) in the safe or failure domain.

Theorem 1 (Set Containment in the Safe Domain). *Let $w(\mathbf{p})$ be the worst-case requirement function defined in (1) and $\rho(\mathcal{H}) = \{\mathcal{R}_1, \dots, \mathcal{R}_t\}$ be a partition of the bounding set \mathcal{H} satisfying $\mathcal{Q} \subseteq \mathcal{H}$. The set containment condition $\mathcal{Q} \subseteq \mathcal{S}$ holds if*

$$\max_{\mathbf{p}} \bar{w}(\mathbf{p}, \rho) < 0. \quad (31)$$

Furthermore, $\mathcal{Q} \not\subseteq \mathcal{S}$ if there exists a $k \leq v$, a $j \leq t$, and a multi-index $\mathbf{i} \in \{0, \mathbf{n}_1\} \times \dots \times \{0, \mathbf{n}_p\}$ such that

$$b_{\mathbf{i}}(\mathcal{R}_j, \mathbf{g}_k) \geq 0. \quad (32)$$

While Formula (31) results from using $\underline{w}(\mathbf{p}) \leq w(\mathbf{p})$ for all $\mathbf{p} \in \mathcal{H}$ in Equation (1), Formula (32) results from applying the free function evaluation property (22).

Theorem 2 (Set Containment in the Failure Domain). *Let $w(\mathbf{p})$ be the worst-case requirement function defined in (1) and $\rho(\mathcal{H}) = \{\mathcal{R}_1, \dots, \mathcal{R}_t\}$ be a partition of the bounding set \mathcal{H} satisfying $\mathcal{Q} \subseteq \mathcal{H}$. The set containment condition $\mathcal{Q} \subseteq \mathcal{F}$ holds if*

$$\min_{\mathbf{p}} \underline{w}(\mathbf{p}, \rho) \geq 0. \quad (33)$$

Furthermore, $\mathcal{Q} \not\subseteq \mathcal{F}$ if there exists a $k \leq v$, a $j \leq t$, and a multi-index $\mathbf{i} \in \{0, \mathbf{n}_1\} \times \dots \times \{0, \mathbf{n}_s\}$ such that

$$b_{\mathbf{i}}(\mathcal{R}_j, \mathbf{g}_k) < 0. \quad (34)$$

While Formula (33) results from using $w(\mathbf{p}) \leq \bar{w}(\mathbf{p})$ for all $\mathbf{p} \in \mathcal{H}$ in Equation (1), Formula (34) results from applying the free function evaluation property (22).

The implicit formulation for calculating Bernstein coefficients proposed in [9] was adopted. This formulation is much more efficient than (12). Further efficiency can be realized by using the subdividing logic in Equation (3) along with the algorithms of [6] that relate the Bernstein coefficients of a hyper-rectangle with those of its subsets.

IV. Uncertainty Quantification in the Presence of Aleatory Uncertainties

In this section we develop strategies for bounding failure probabilities, means and variances of response metrics that depend exclusively on aleatory uncertain parameters.

A. Reliability Analysis

By reliability analysis we refer to the bounding of the probability of failure. The key developments in this section are the calculation of inner and outer bounding sets to the failure domain and the calculation of their probabilities. These sets are comprised by hyper-rectangles whose membership into the bounding set is established using Theorems 1 and 2. Bernstein expansion-based techniques and interval analysis-based techniques⁵ can be used to calculate these sets. The sets resulting from the latter technique however, are considerably more slack than those of the alternative technique for the same number of subsets. Furthermore, Bernstein bounds can always be made to converge to the function/set being bounded while bounds based on interval arithmetic may not, e.g. cases where the requirement functions have repeated parameters.

This section presents an algorithm to generate and sequentially expand subsets of the failure and safe domains. These sets are unions of disjoint hyper-rectangles chosen from a partition ρ of \mathcal{D} . Let \mathcal{F}^{sub} and \mathcal{S}^{sub} denote subsets (i.e., inner approximations) of the failure and safe domains formed from selected elements of ρ . Note that $\emptyset \subseteq \mathcal{F}^{\text{sub}} \subseteq \mathcal{F} \subseteq C(\mathcal{S}^{\text{sub}}) \subseteq \mathcal{D}$ and that the failure domain boundary, denoted as $\partial\mathcal{F}$, lies in the region between the interiors of \mathcal{F}^{sub} and \mathcal{S}^{sub} .

The sequences of inner bounding sets $\{\mathcal{S}_1^{\text{sub}}, \mathcal{S}_2^{\text{sub}}, \dots\}$ and $\{\mathcal{F}_1^{\text{sub}}, \mathcal{F}_2^{\text{sub}}, \dots\}$ are generated by the algorithm below. These sequences are made to converge to the domain being bounded. In particular, the algorithm iteratively generates indexed partitions Q_i of \mathcal{D} and indexed sets $\mathcal{S}_i^{\text{sub}}$, $\mathcal{F}_i^{\text{sub}}$ and Λ_i which are unions of hyper-rectangles from Q_i , where $\mathcal{S}_i^{\text{sub}}$ is an inner approximation to the safe domain, $\mathcal{F}_i^{\text{sub}}$ is an inner approximation to the failure domain, and Λ_i is a region comprised by the rectangles of Q_i that are not in $\mathcal{S}_i^{\text{sub}}$ or $\mathcal{F}_i^{\text{sub}}$. Note that while Q_i is a list of hyper-rectangles, $\mathcal{S}_i^{\text{sub}}$, $\mathcal{F}_i^{\text{sub}}$ and Λ_i are sets comprised by the union of some of these rectangles. The algorithm proceeds by successively selecting each of the component hyper-rectangles \mathcal{R} of Λ_i . Then, Theorems 1 and 2 are used to determine if \mathcal{R} is contained by the failure or safe domains. If the tests determine that $\mathcal{R} \subseteq \mathcal{S}$ or $\mathcal{R} \subseteq \mathcal{F}$, then \mathcal{R} is removed from Λ_i and added to $\mathcal{S}_i^{\text{sub}}$ or $\mathcal{F}_i^{\text{sub}}$, respectively. If neither of these conditions is satisfied, \mathcal{R} is subdivided, and the resulting sub-rectangles replace \mathcal{R} in the partition. The algorithm terminates when the volume of Λ_i is sufficiently small.

The algorithmic representation of this procedure is as follows. Let the inequality constraint $\mathbf{g}(\mathbf{p}) < \mathbf{0}$ over $\mathbf{p} \in \mathcal{D}$ prescribe the system requirements. Set $i = 1$, $Q_1 = \{\mathcal{D}\}$, $\Lambda_1 = \mathcal{D}$, $\mathcal{F}_1^{\text{sub}} = \emptyset$, and $\mathcal{S}_1^{\text{sub}} = \emptyset$. Pick a convergence criterion $\epsilon > 0$.

1. Let L contain the elements of Q_i comprising Λ_i .
2. Apply Theorems 1 and 2 to each hyper-rectangle in L without partitioning it, to determine which elements of L are contained in the safe domain and which ones are contained in the failure domain. Denote by U the list of elements contained by the safe domain, by V the list of elements contained by the failure domain, and by W the

list of elements that are not in U nor V . Furthermore, let \mathcal{U} , \mathcal{V} and \mathcal{W} be the union of the elements in U , V and W respectively.

3. Make $\mathcal{S}_{i+1}^{\text{sub}} = \mathcal{S}_i^{\text{sub}} \cup \mathcal{U}$; $\mathcal{F}_{i+1}^{\text{sub}} = \mathcal{F}_i^{\text{sub}} \cup \mathcal{V}$; and $\Lambda_{i+1} = \Lambda_i \setminus (\mathcal{U} \cup \mathcal{V})$.
4. If $\text{Vol}(\Lambda_{i+1}) < \epsilon$ stop. Otherwise, make $Q_{i+1} = (Q_i \setminus W) \cup \rho(W)$, increase i by one, and go to Step (1).

As the number of iterations increases, $\mathcal{S}_i^{\text{sub}}$ and $\mathcal{F}_i^{\text{sub}}$ approach the safe and failure domain. Notice that the subdividing algorithm only partitions boxes whose containment in \mathcal{S} or in \mathcal{F} has not been established. Further notice that the closure of Λ_i not only covers the boundary of \mathcal{F} but also approaches that boundary more and more closely as i increases.

If a particular CDF defined over $\mathbf{p} \in \Delta \subseteq \mathcal{D}$ is prescribed, bounds to the failure probability, given by

$$P[\mathcal{F}_i^{\text{sub}}] \leq P[\mathcal{F}] \leq 1 - P[\mathcal{S}_i^{\text{sub}}], \quad (35)$$

can be readily calculated. These expressions are evaluated by adding up the probability of the rectangles comprising the bounding sets. Note that $P[\mathcal{F}_i^{\text{sub}}]$ and $P[\mathcal{S}_i^{\text{sub}}]$ are monotonically increasing functions of i ; while $P[\Lambda_i]$ is a monotonically decreasing function of i . The choice of \mathcal{R} made at step 1 of the algorithm implies that these bounds converge to $P_F[\mathcal{F}]$ as i increases. Therefore, all the conservatism in the bounds is reducible by additional computational effort. Further notice that once the bounding sets are available, failure probability bounds corresponding to any distribution supported in a subset of \mathcal{D} can be calculated efficiently.

The values taken by \underline{w} and \bar{w} over the members of the partition ρ , which were required to compute the bounding sets \mathcal{S}^{sub} and \mathcal{F}^{sub} , can be used to bound the CDF of the worst-case requirement function w . In particular, if $\rho(\mathcal{D}) = \{\mathcal{R}_1, \dots, \mathcal{R}_t\}$, F_w is bounded by

$$F_{\bar{w}}(x) = \sum_{j \in \bar{j}(x)} P[\mathcal{R}_j] \leq F_w(x) \leq \sum_{j \in \underline{j}(x)} P[\mathcal{R}_j] = F_{\underline{w}}(x), \quad (36)$$

where $\bar{j}(x) = \{j : 1 \leq j \leq t, \bar{w}(\mathbf{p}^{(j)}) \leq x\}$ and $\underline{j}(x) = \{j : 1 \leq j \leq t, \underline{w}(\mathbf{p}^{(j)}) \leq x\}$ for all x in the range of w . A few manipulations lead to

$$1 - F_{\underline{w}}(0) \leq P[\mathcal{F}] \leq 1 - F_{\bar{w}}(0). \quad (37)$$

This expression is equivalent to (35). The evaluation of (36) for each member of the partition sequence Q_i resulting from the algorithm above yields a sequence of CDF bounds. These CDFs become tighter near $w = 0$ as i increases.

Example 1: Consider the requirement functions

$$\mathbf{g}_1 = \mathbf{p}_1^2 \mathbf{p}_2^4 + \mathbf{p}_1^4 \mathbf{p}_2^2 - 3\mathbf{p}_1^2 \mathbf{p}_2^2 - \mathbf{p}_1 \mathbf{p}_2 + \frac{\mathbf{p}_1^6 + \mathbf{p}_2^6}{200} - \frac{7}{100}, \quad (38)$$

$$\mathbf{g}_2 = -\frac{\mathbf{p}_1^2 \mathbf{p}_2^4}{2} - \mathbf{p}_1^4 \mathbf{p}_2^2 + 3\mathbf{p}_1^2 \mathbf{p}_2^2 + \frac{\mathbf{p}_1^5 \mathbf{p}_2^3}{10} - \frac{9}{10}, \quad (39)$$

defined over the master domain $\mathcal{D} \in [-2, 2] \times [-2, 2]$. The parameters \mathbf{p}_1 and \mathbf{p}_2 are aleatory uncertain parameters, i.e., $\mathbf{a} = \{\mathbf{p}_1, \mathbf{p}_2\}$ and $\mathbf{e} = \emptyset$, distributed according to the PDF

$$f_{\mathbf{p}_1 \mathbf{p}_2}(\mathbf{p}_1, \mathbf{p}_2) = \frac{\cos^2(\mathbf{p}_1 \mathbf{p}_2)}{8 + \text{Si}(8)}, \quad (40)$$

where $\text{Si}(\cdot)$ is the sine integral. Note that the uncertainty models of \mathbf{p}_1 and \mathbf{p}_2 are strongly dependent. For instance, the conditional probability density function of \mathbf{p}_1 given \mathbf{p}_2 is uniform at $\mathbf{p}_2 = 0$, and it is tri-modal at $\mathbf{p}_2 = -2$.

Figure 1 shows the set approximations \mathcal{F}_i^{sub} and \mathcal{S}_i^{sub} for a fixed value of i . Boxes comprising \mathcal{F}_i^{sub} are colored in red, those comprising \mathcal{S}_i^{sub} are colored in green, and boxes comprising Λ_i are colored in white. Note that Λ_i is a tight approximation of $\partial\mathcal{F}$. Further notice that the density of boxes per unit of area increases with the closeness to $\partial\mathcal{F}$. The

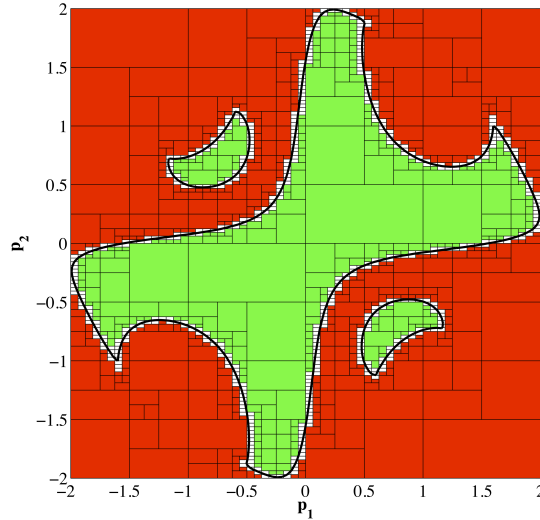


Figure 1. \mathcal{F}^{sub} (red) and \mathcal{S}^{sub} (green) and failure domain boundary (thick line).

corresponding failure probability bounds are $0.492 \leq P[\mathcal{F}] \leq 0.571$. This probability cannot be calculated by standard sampling techniques.

B. Performance Analysis

Lower and upper bounds of moments of any performance function that depends on aleatory variables can be calculated from Equation (23). If the performance function g is a single polynomial in \mathbf{p} and the aleatory parameters are independent random variables, moments of any order can be calculated exactly. This is not the case when either g is a continuous piecewise polynomial function, or when the aleatory variables are not independently distributed.

In this section we develop techniques for bounding $E[g(\mathbf{p})]$ and $V[g(\mathbf{p})]$ when \mathbf{g} is piecewise polynomial, and \mathbf{p} is arbitrary distributed within a bounded set. The application of such techniques requires the calculation of the bounding functions in Equation (23). Even though the approach is applicable to any partition of the master domain, tighter bounds are obtained when the partition is finer in regions where either $\bar{g} - \underline{g}$ or $E[\bar{g} - \underline{g}|\mathcal{R}]$ are large.

In regard to the mean, the application of the expected value operator to Equation (23)

yields

$$\sum_{j=1}^t \underline{g}(\mathbf{p}^{(j)})P[\mathcal{R}_j] \leq E[g] \leq \sum_{j=1}^t \bar{g}(\mathbf{p}^{(j)})P[\mathcal{R}_j]. \quad (41)$$

Bounds on the variance are considered next. Interval arithmetic will be used to simplify the notation. The starting point is the equation $V[g] = E[g^2] - E[g]^2$ and the interval inclusion $g \in [\underline{g}, \bar{g}]$. We recall the formulae for interval subtraction and interval squaring: $[a, b] - [c, d] \triangleq [a - d, b - c]$ and

$$[a, b]^2 \triangleq \begin{cases} [a^2, b^2] & \text{if } 0 < a, \\ [b^2, a^2] & \text{if } b < 0, \\ [0, \max\{a^2, b^2\}] & \text{otherwise.} \end{cases} \quad (42)$$

In this context, $g^2 \in [\underline{g}, \bar{g}]^2$ and $E[g^2] \in E[[\underline{g}, \bar{g}]^2] = [\mu, \nu]$. The evaluation of this equation yields

$$\mu = \sum_{j \in U} \underline{g}(\mathbf{p}^{(j)})^2 P[\mathcal{R}_j] + \sum_{j \in V} \bar{g}(\mathbf{p}^{(j)})^2 P[\mathcal{R}_j], \quad (43)$$

$$\nu = \sum_{j \in U \cup W} \bar{g}(\mathbf{p}^{(j)})^2 P[\mathcal{R}_j] + \sum_{j \in V \cup X} \underline{g}(\mathbf{p}^{(j)})^2 P[\mathcal{R}_j], \quad (44)$$

where

$$U = \{1 \leq j \leq t : \underline{g}(\mathbf{p}^{(j)}) \geq 0\}, \quad (45)$$

$$V = \{1 \leq j \leq t : \bar{g}(\mathbf{p}^{(j)}) < 0\}, \quad (46)$$

$$W = \{1 \leq j \leq t : \underline{g}(\mathbf{p}^{(j)})\bar{g}(\mathbf{p}^{(j)}) < 0, |\underline{g}(\mathbf{p}^{(j)})| \leq |\bar{g}(\mathbf{p}^{(j)})|\}, \text{ and} \quad (47)$$

$$X = \{1 \leq j \leq t : j \notin (U \cup V \cup W)\}. \quad (48)$$

The desired bounds are given by $V[g] \in E[[\underline{g}, \bar{g}]^2] - [E[\underline{g}], E[\bar{g}]]^2$, whose evaluation yields

$$\max\{0, \alpha\} \leq V[g] \leq \beta, \quad (49)$$

where

$$\alpha = \begin{cases} \mu - E[\bar{g}]^2 & \text{if } E[\underline{g}] > 0, \\ \mu - E[\underline{g}]^2 & \text{if } E[\bar{g}] < 0, \\ \mu - \max\{E[\underline{g}]^2, E[\bar{g}]^2\} & \text{otherwise,} \end{cases} \quad (50)$$

$$\beta = \begin{cases} \nu - E[\underline{g}]^2 & \text{if } E[\underline{g}] > 0, \\ \nu - E[\bar{g}]^2 & \text{if } E[\bar{g}] < 0, \\ \nu & \text{otherwise.} \end{cases} \quad (51)$$

Example 2: Given the same problem statement of Example 1, we want to bound $E[w]$

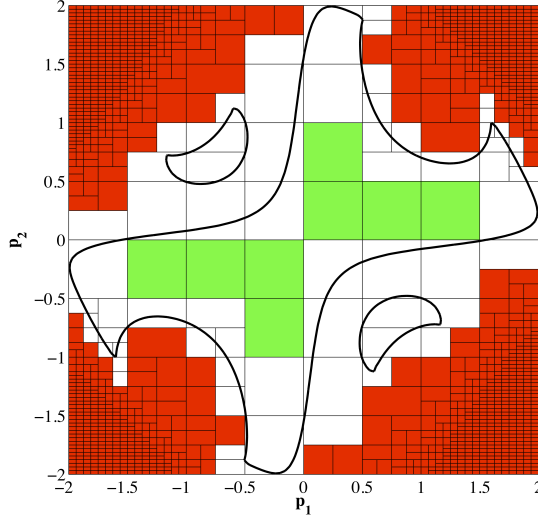


Figure 2. \mathcal{F}^{sub} (red) and \mathcal{S}^{sub} (green) and failure domain boundary (thick line).

and $V[w]$, where w is the worst-case requirement function. Figures 2 and 3 show the set approximations \mathcal{F}_i^{sub} and \mathcal{S}_i^{sub} for a fixed value of i corresponding to two partition logics. The partition used to generate Figure 2 only subdivides boxes where $\bar{g} - \underline{g}$ is in the top 50%. This partition leads to $3.21052 \leq E[w] \leq 4.71449$ and $80.97456 \leq V[w] \leq 145.11712$. In this case, the density of boxes per unit of area increases with the separation between the upper and lower bounds of w . This separation is an indicator of the size of the range of w over a box. Consequently, the size of a box tends to be inversely proportional to the magnitude of the gradient of w within the box. Note that the determination of whether a given box is in the failure or safe domain, therefore the coloring of the boxes in the figure, is inconsequential.

The partition used to generate Figure 3 only subdivides boxes where $E[\bar{g} - \underline{g} | \mathcal{R}]$ is in the top 50%. This yields $3.40700 \leq E[w] \leq 4.50007$ and $82.9050 \leq V[w] \leq 143.5641$. This set of bounds are tighter than those from Figure 2 because they take into account the uncertainty model. In this case, the size of a box tends to be inversely proportional to the magnitude of the probability-weighted gradient of w within the box.

V. Uncertainty Quantification in the Presence of Aleatory and Epistemic Uncertainties

In this section we develop strategies for bounding failure probabilities, means and variances of response metrics that depend on both aleatory and epistemic parameters. Recall that the propagation of probabilistic uncertainty from the aleatory variables to the response metrics yields a random process whose statistics are parametrized by the epistemic variables. Note that for a fixed value of the epistemic variable, the UQ methods of Section IV apply. While for the aleatory-only case the statistics take on a constant value, taking into account the epistemic intervals of uncertainty spreads each aleatory statistic over its own interval of

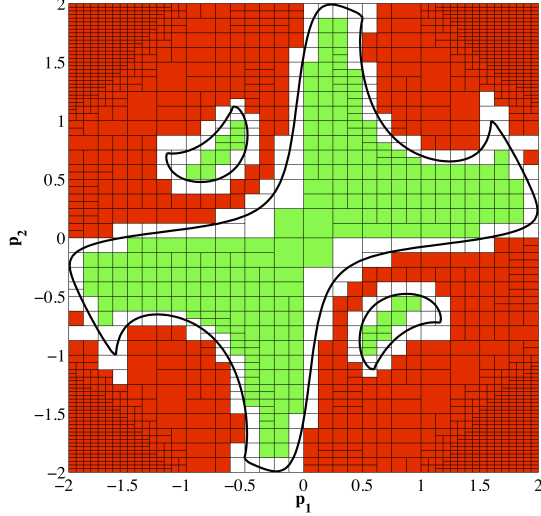


Figure 3. \mathcal{F}^{sub} (red) and \mathcal{S}^{sub} (green) and failure domain boundary (thick line).

uncertainty. Each value in that interval is a possible realization of the statistic. The values of the epistemic realizations prescribing the interval's limits will be referred to as best-case and worst-case epistemic values. These values will be denoted hereafter as \mathbf{e}_* and \mathbf{e}^* . In this section we use the Bernstein expansion approach to bound the range statistics of the response metric and calculate supersets of the corresponding \mathbf{e}_* and \mathbf{e}^* . The mathematical background for this is presented next.

Denote by $\text{Proj}_{\mathbf{a}}(\mathcal{X})$ the projection of the set $\mathcal{X} \subseteq \mathbb{R}^s$ onto the aleatory subspace and by $\text{Proj}_{\mathbf{e}}(\mathcal{X})$ its projection onto the epistemic subspace. Note that $\mathcal{D}_{\mathbf{e}} = \text{Proj}_{\mathbf{e}}(\mathcal{D})$ and $\mathcal{D}_{\mathbf{a}} = \text{Proj}_{\mathbf{a}}(\mathcal{D})$. While the aleatory uncertainty is fully prescribed by a PDF whose support set is a subset of $\mathcal{D}_{\mathbf{a}}$, the epistemic variable is prescribed by a subset of $\mathcal{D}_{\mathbf{e}}$. In this context, $w(\mathbf{a}, \mathbf{e}) = \max_{i \leq v} \{g_i(\mathbf{a}, \mathbf{e})\}$ is the worst-case requirement function.

A. Reliability Analysis

The reliability analysis of a system subject to the design requirements $\mathbf{g}(\mathbf{a}, \mathbf{e}) < \mathbf{0}$ consists of determining

$$\text{Range}(P[\mathcal{F}(\mathbf{e})]) = \left[\min_{\mathbf{e} \in \Delta_{\mathbf{e}}} P[w(\cdot, \mathbf{e}) > 0], \max_{\mathbf{e} \in \Delta_{\mathbf{e}}} P[w(\cdot, \mathbf{e}) > 0] \right], \quad (52)$$

and calculating the epistemic point(s) that realize this interval's limits. The range enclosing property (23) becomes

$$\underline{w}(\mathbf{a}, \mathbf{e}, \rho) \leq w(\mathbf{a}, \mathbf{e}) \leq \bar{w}(\mathbf{a}, \mathbf{e}, \rho). \quad (53)$$

As before, ρ is a partition of the master domain $\mathcal{D} = \mathcal{D}_{\mathbf{a}} \times \mathcal{D}_{\mathbf{e}}$. A few manipulations lead to

$$P[\underline{w}(\mathbf{a}, \mathbf{e}, \rho) > 0] \leq P[\mathcal{F}(\mathbf{e})] \leq P[\bar{w}(\mathbf{a}, \mathbf{e}, \rho) > 0], \quad (54)$$

which is equivalent to

$$1 - F_{\underline{w}}(0; \mathbf{e}) \leq P[\mathcal{F}(\mathbf{e})] \leq 1 - F_{\overline{w}}(0; \mathbf{e}), \quad (55)$$

where $F_x(\cdot; \mathbf{e})$ is the CDF of $x(\cdot; \mathbf{e})$. Lower and upper bounds to $F_w(\cdot; \mathbf{e})$, which are parametrized by \mathbf{e} , are given by

$$F_{\overline{w}}(x; \mathbf{e}) \leq F_w(x; \mathbf{e}) \leq F_{\underline{w}}(x; \mathbf{e}). \quad (56)$$

Details on the evaluation of Equations (55) and (56) are presented next. Assume that $\rho(\mathcal{D})$ is a partition of the master domain resulting from the algorithm in Section IV-A. In this case the hyper-rectangles comprising the partition are supported in both the epistemic and aleatory spaces. Subdivisions in the aleatory dimensions will tighten the probability bounds while subdivisions in the epistemic dimensions will tighten the supersets containing the best- and worst-case epistemic realizations. The evaluation of the CDF bounds in Equation (56) yields

$$\sum_{j \in \overline{J}(x, \mathbf{e})} P[\text{Proj}_{\mathbf{a}}(\mathcal{R}_j)] \leq F_w(x; \mathbf{e}) \leq \sum_{j \in \underline{J}(x, \mathbf{e})} P[\text{Proj}_{\mathbf{a}}(\mathcal{R}_j)], \quad (57)$$

where first $J(\mathbf{e}) = \{j : 1 \leq j \leq t \text{ and } \mathbf{e} \in \text{Proj}_{\mathbf{e}}(\mathcal{R}_j)\}$ contains the indices of the members of the partition $\rho(\mathcal{D})$ whose projection onto the epistemic subspace contains the epistemic realization \mathbf{e} , and then $\overline{J}(x, \mathbf{e}) = \{j \in J(\mathbf{e}) : \overline{w}(\mathbf{p}^{(j)}) \leq x\}$ and $\underline{J}(x, \mathbf{e}) = \{j \in J(\mathbf{e}) : \underline{w}(\mathbf{p}^{(j)}) \leq x\}$ pick out those members of the partition which contribute to the respective CDFs. Note the similarity between Equations (36) and (57). The evaluation of Equation (57) at $x = 0$ leads to Equation (55).

The bounds in Equation (57) enable determining an outer bounding interval to the failure probability range

$$\text{Range}(P[\mathcal{F}(\mathbf{e})]) \subseteq [1 - \max_{\mathbf{e} \in \Delta_{\mathbf{e}}} F_{\underline{w}}(0; \mathbf{e}), 1 - \min_{\mathbf{e} \in \Delta_{\mathbf{e}}} F_{\overline{w}}(0; \mathbf{e})]. \quad (58)$$

Since \underline{w} and \overline{w} are piecewise constant on a finite partition of Δ , the extrema in Equation (58) can be determined exactly in a finite number of steps.

Supersets of \mathbf{e}_* and \mathbf{e}^* , where such extrema occur, are given by

$$\mathcal{E}_* = \bigcup_{j \in \underline{J}(0, \mathbf{e})} \left\{ \text{Proj}_{\mathbf{e}}(\mathcal{R}_j) : F_{\underline{w}}(0; \mathbf{e}) \geq \max_{\mathbf{e}} F_{\overline{w}}(0; \mathbf{e}) \right\} \supset \mathbf{e}_*, \quad (59)$$

$$\mathcal{E}^* = \bigcup_{j \in \overline{J}(0, \mathbf{e})} \left\{ \text{Proj}_{\mathbf{e}}(\mathcal{R}_j) : F_{\overline{w}}(0; \mathbf{e}) \leq \min_{\mathbf{e}} F_{\underline{w}}(0; \mathbf{e}) \right\} \supset \mathbf{e}^*. \quad (60)$$

The inequalities in these expressions result from combining Equations (27-28) and (55). Equation (57) enables evaluating these inequalities. Observe that the subsets $\text{Proj}_{\mathbf{e}}(\mathcal{R}_j)$ of $\mathcal{D}_{\mathbf{e}}$, can be used to generate a partition of $\mathcal{D}_{\mathbf{e}}$ into finitely many pieces, on each of which $F_{\underline{w}}(0; \mathbf{e})$ and $F_{\overline{w}}(0; \mathbf{e})$ is constant. Equation (58) converges to (52) while \mathcal{E}_* , and \mathcal{E}^* converge to \mathbf{e}_* and \mathbf{e}^* when the volume of Λ approaches zero.

The algorithmic implementation of the above ideas has the very same structure of the algorithm in Section IV-A. Only two minor variations are required. First, at Step 1, \mathcal{R} will now be the largest element of Λ_i that satisfies $\text{Proj}_{\mathbf{e}}(\mathcal{R}) \in \mathcal{E}_* \cup \mathcal{E}^*$. This will ensure that only

those regions of the epistemic space where the best- and worst-case realizations may be located are partitioned further. Second, at Step 5, the new stopping criterion could be given by $\text{Volume}[\mathcal{E}_* \cup \mathcal{E}^*]$ being smaller than a prescribed constant, or by having a sufficiently small change in the size of the bounding interval in Equation (58). The former criterion implies that the supersets are sufficiently small, while the latter implies tight bounds on the extrema.

Example 3: Consider the requirement functions

$$\mathbf{g}_1 = -3\mathbf{p}_1^2\mathbf{p}_2^5 + 3\mathbf{p}_1^2 - \mathbf{p}_2^2 - 4\mathbf{p}_2 - 15, \quad (61)$$

$$\mathbf{g}_2 = -\mathbf{p}_1^{11}\mathbf{p}_2 + \mathbf{p}_1^2\mathbf{p}_2^7 - \frac{1}{10}, \quad (62)$$

$$\mathbf{g}_3 = -2\mathbf{p}_1^4 - \mathbf{p}_2^6 - \mathbf{p}_1^2\mathbf{p}_2 - \frac{\mathbf{p}_1\mathbf{p}_2^5}{10} + \frac{1}{500}, \quad (63)$$

defined over the master domain $\mathcal{D} \in [-2, 2] \times [-2, 2]$.

To start, \mathbf{p}_1 will be considered a Beta-distributed aleatory variable with parameters $\langle 4, 4 \rangle$ in $[-2, 2]$ while \mathbf{p}_2 will be epistemic in $[-2, 2]$. Therefore, $\mathbf{a} = \{\mathbf{p}_1\}$, $\mathbf{e} = \{\mathbf{p}_2\}$ and $\Delta = \mathcal{D}$. In this setting we would like to bound the extrema of $P[\mathcal{F}]$ and calculate supersets of the corresponding best- and worst- case epistemic values. Figure 4 shows the supersets \mathcal{E}^* and \mathcal{E}_* of the worst- and best-case epistemic realizations as a function of the iteration number. This figure illustrates how the supersets are progressively refined. In both cases, there seems to be a single extrema. The existence of an isolated region in the vicinity of $\mathbf{p}_2 = 0$ for \mathcal{E}^* at iteration number 8 and of $\mathbf{p}_1 = 0.39$ for \mathcal{E}_* at iteration number 14, and their subsequent disappearance, suggests the existence of local maxima. Figure 5 shows the corresponding

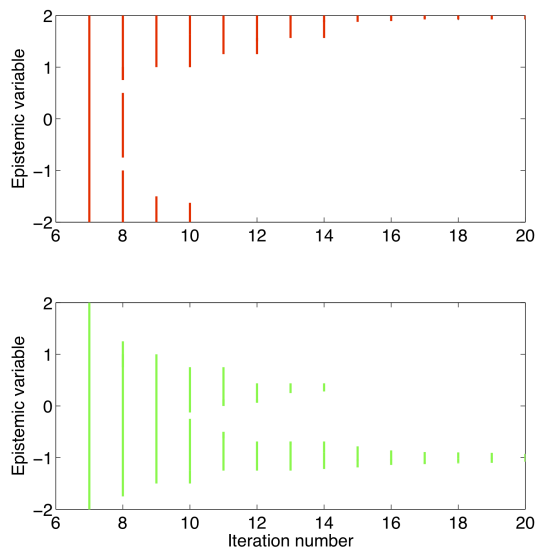


Figure 4. Sequence of \mathcal{E}^* (upper graph) and \mathcal{E}_* (lower graph) for $\mathbf{a} = \{\mathbf{p}_1\}$ and $\mathbf{e} = \{\mathbf{p}_2\}$.

partition of the parameter space. Note that Λ , the region containing the failure domain boundary colored in white, has not been uniformly refined. Further notice that the density of boxes increases with the proximity to the extrema of $P[\mathcal{F}(\mathbf{e})]$. These extrema occur within

$\mathcal{E}^* = [1.9336, 2]$ and $\mathcal{E}_* = [-1.07, -0.941]$ at iteration $i = 20$. The top of Figure 6 shows the

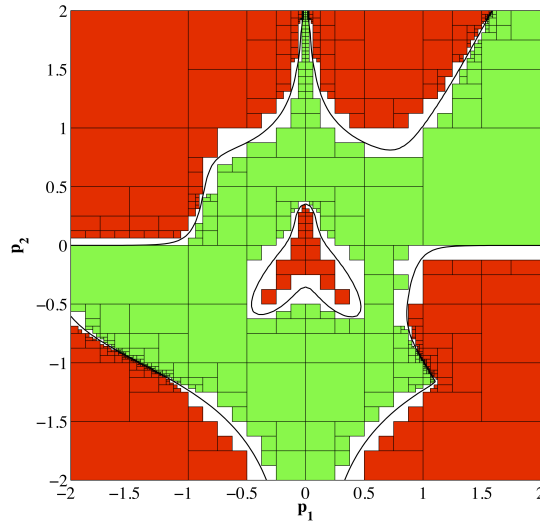


Figure 5. Partition of the uncertain parameter space for $a = \{p_1\}$ and $e = \{p_2\}$.

probability of Λ as a function of the epistemic variable p_2 . The bottom of this figure shows the failure probability bounds over the epistemic domain. Note that $P[\Lambda]$ approaches zero in the vicinity of the points where the best- and worst- case epistemic values occur. Values of p_2 where $P[\Lambda]$ is comparatively large are regions of no interest. The supersets \mathcal{E}_* and \mathcal{E}^* corresponding to the last iteration in Figure 4 are superimposed in Figure 6. Finally, Figure

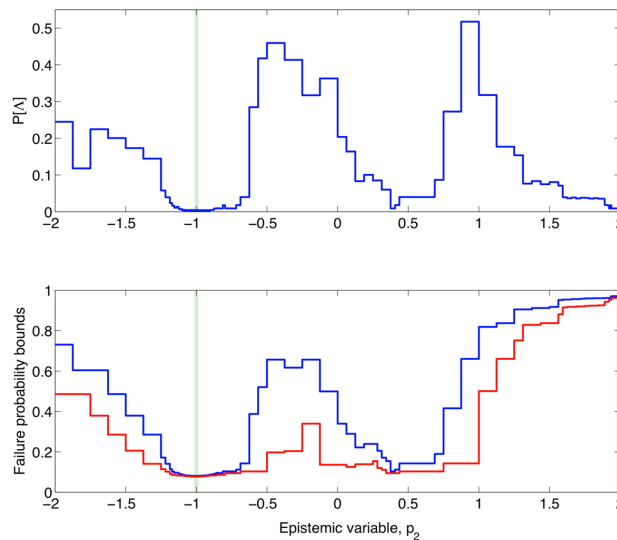


Figure 6. Probability of Λ and bounds of $P[\mathcal{F}]$ for $a = \{p_1\}$ and $e = \{p_2\}$.

7 shows the ensemble of all CDF bounds, as well as bounds corresponding to epistemic

values in \mathcal{E}_* and \mathcal{E}^* . While the lower bound of the worst-case representative crosses $w = 0$ at $F_w(0; \mathbf{e}) = 1 - 0.076931$, the upper bound of the best-case representative crosses $w = 0$ at $F_{\bar{w}}(0; \mathbf{e}) = 1 - 0.97148$. Hence, the bounding interval of the failure probability range is $[0.076931, 0.97148]$. Note that the separation between the lower and upper CDF bounds decreases with the proximity to $w = 0$.

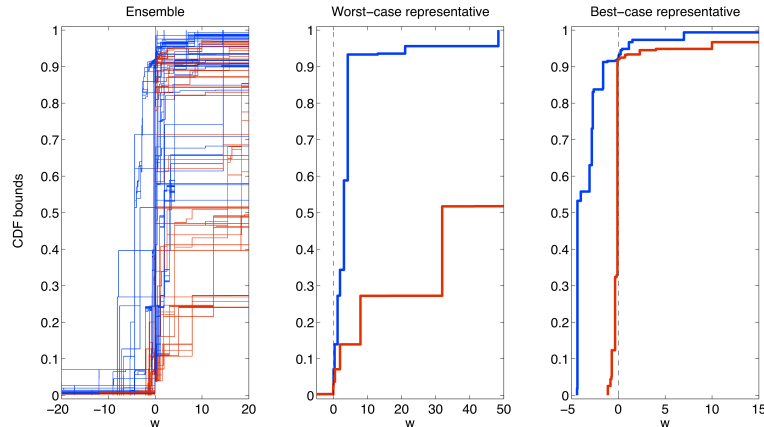


Figure 7. Ensemble of CDF bounds, worst- and best-case CDF bounds representatives for $\mathbf{a} = \{\mathbf{p}_1\}$ and $\mathbf{e} = \{\mathbf{p}_2\}$.

We will now repeat this example by considering \mathbf{p}_1 as an epistemic variable while \mathbf{p}_2 will be an aleatory variable having a Beta PDF with parameters $\langle 4, 6 \rangle$ such that $\Delta = \mathcal{D}$. Therefore $\mathbf{a} = \{\mathbf{p}_2\}$ and $\mathbf{e} = \{\mathbf{p}_1\}$. Figure 8 shows the supersets \mathcal{E}^* and \mathcal{E}_* of the worst- and best-case epistemic realizations as a function of the iteration number. In contrast to the previous example, the \mathcal{E}_* sequence suggests the existence of two global minima. Recall that the exact nature of the approach guarantees that all global extrema will be found. Figure 9 shows the corresponding partition of the parameter space. Note that the density of boxes in λ increases with the proximity to $\mathcal{E}^* = [1.2578, 2]$ and $\mathcal{E}_* = [-0.48434, -0.46094] \cup [0.46094, 0.48434]$. These are the supersets of the best- and worst-case epistemic realizations at iteration 20. Figure 10 and 11 are analogous to Figures 6 and 7. While the lower bound of the worst-case representative crosses $w = 0$ at $F_w(0; \mathbf{e}) = 1 - 0.01792$, the upper bound of the best-case representative crosses $w = 0$ at $F_{\bar{w}}(0; \mathbf{e}) = 1 - 0.74623$. Hence, the bounding interval of the failure probability range is $[0.01792, 0.74623]$.

B. Performance Analysis

$E[g(\mathbf{a}, \mathbf{e})]$ and $V[g(\mathbf{a}, \mathbf{e})]$ can be calculated analytically when the aleatory parameters are independent random variables and g is a single polynomial. In such a case one can solve for the corresponding extrema and the best- and worst- case realizations by performing the analysis of Section III to the resulting expressions. These expressions will be polynomials in \mathbf{e} . If g is a piecewise polynomial function of \mathbf{p} (e.g., the worst-case requirements function w) and the aleatory parameters are arbitrarily dependent random variables, an approach analogous to the one in the preceding section can be applied.

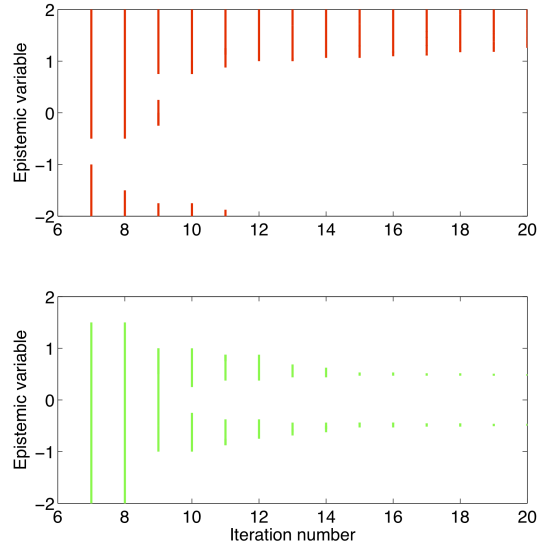


Figure 8. Sequence of \mathcal{E}^* (upper graph) and \mathcal{E}_* (lower graph) for $a = \{p_2\}$ and $e = \{p_1\}$.

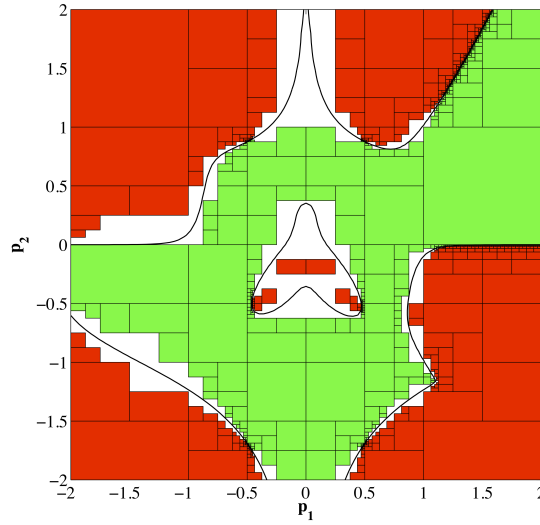


Figure 9. Partition of the uncertain parameter space for $a = \{p_2\}$ and $e = \{p_1\}$.

An outer bounding interval to the range of expected values is given by

$$\text{Range}(E[g(\cdot, e)]) \subseteq \left[\min_{e \in \Delta_e} E[\underline{g}(\cdot, e)], \max_{e \in \Delta_e} E[\bar{g}(\cdot, e)] \right], \quad (64)$$

where

$$E[\underline{g}(\cdot, e)] = \sum_{j \in J(e)} \underline{g}(\mathbf{p}^{(j)}) P[\text{Proj}_a(\mathcal{R}_j)], \quad (65)$$

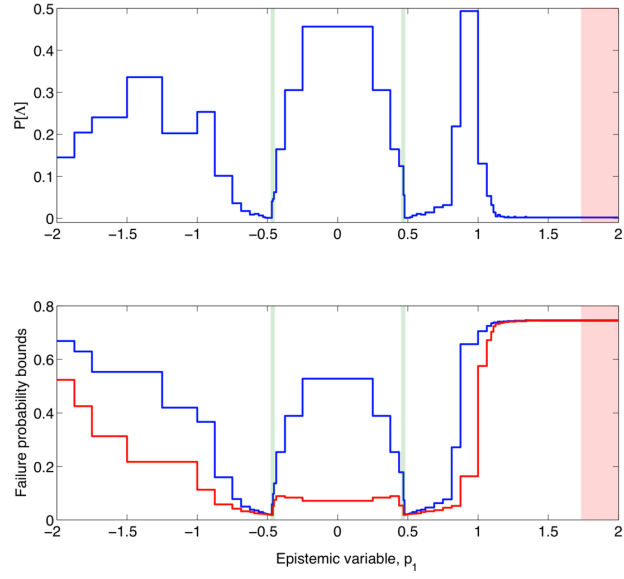


Figure 10. Probability of Λ and bounds of $P[\mathcal{F}]$ for $\mathbf{a} = \{p_2\}$ and $\mathbf{e} = \{p_1\}$.

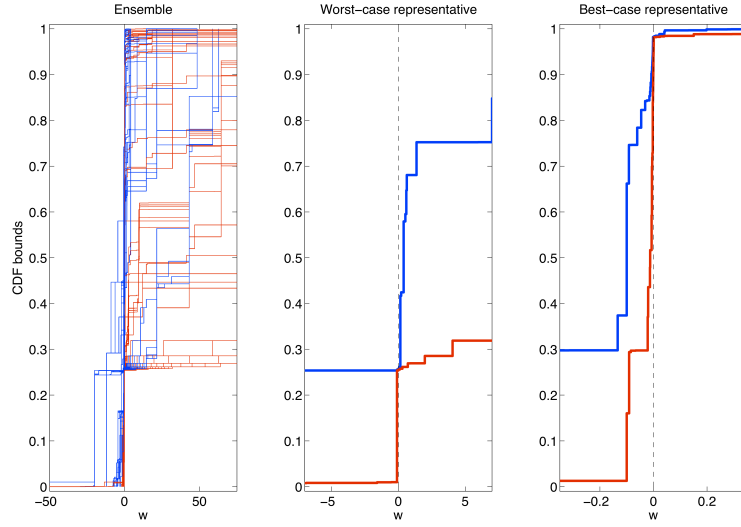


Figure 11. Ensemble of CDF bounds, worst- and best-case CDF bounds representatives for $\mathbf{a} = \{p_2\}$ and $\mathbf{e} = \{p_1\}$.

$$E[\bar{g}(\cdot, \mathbf{e})] = \sum_{j \in J(\mathbf{e})} \bar{g}(\mathbf{p}^{(j)}) P[\text{Proj}_{\mathbf{a}}(\mathcal{R}_j)], \quad (66)$$

and $J(\mathbf{e}) = \{j : 1 \leq j \leq t, \mathbf{e} \in \text{Proj}_{\mathbf{e}}(\mathcal{R}_j)\}$. Supersets of the epistemic realizations prescrib-

ing the endpoints of $E[\underline{g}(\cdot, \mathbf{e})]$ are

$$\mathcal{E}_* = \bigcup_{j \in J(\mathbf{e})} \left\{ \text{Proj}_e(\mathcal{R}_j) : E[\underline{g}(\cdot, \mathbf{e})] \leq \min_e E[\underline{g}] \right\} \supset \mathbf{e}_*, \quad (67)$$

$$\mathcal{E}^* = \bigcup_{j \in J(\mathbf{e})} \left\{ \text{Proj}_e(\mathcal{R}_j) : E[\bar{g}(\cdot, \mathbf{e})] \geq \max_e E[\bar{g}] \right\} \supset \mathbf{e}^*. \quad (68)$$

Equations (65) and (66) enable evaluating the inequality constraints in Equations (67) and (68).

An outer bounding interval of the variance is

$$\text{Range}(V[g(\cdot, \mathbf{e})]) \subseteq [\max\{0, \alpha(\mathbf{e})\}, \beta(\mathbf{e})], \quad (69)$$

where $\alpha(\mathbf{e})$ and $\beta(\mathbf{e})$ are given by Equations (50) and (51) with the expected values given by Equations (65) and (66), and with $\mu(\mathbf{e})$ and $\nu(\mathbf{e})$ given by

$$\mu(\mathbf{e}) = \sum_{j \in U(\mathbf{e})} \underline{g}(\mathbf{p}^{(j)})^2 P[\text{Proj}_a(\mathcal{R}_j)] + \sum_{j \in V(\mathbf{e})} \bar{g}(\mathbf{p}^{(j)})^2 P[\text{Proj}_a(\mathcal{R}_j)], \quad (70)$$

$$\nu(\mathbf{e}) = \sum_{j \in U(\mathbf{e}) \cup W(\mathbf{e})} \bar{g}(\mathbf{p}^{(j)})^2 P[\text{Proj}_a(\mathcal{R}_j)] + \sum_{j \in V(\mathbf{e}) \cup X(\mathbf{e})} \underline{g}(\mathbf{p}^{(j)})^2 P[\text{Proj}_a(\mathcal{R}_j)], \quad (71)$$

where U , V , W and X are defined in Equations (45-48) and $\mathbf{e} \in \text{Proj}_e(\mathcal{R}_j)$. Supersets of the epistemic realizations where the extreme values of $V[g(\cdot, \mathbf{e})]$ occur are

$$\mathcal{E}_* = \bigcup_{j \in J(\mathbf{e})} \left\{ \text{Proj}_e(\mathcal{R}_j) : \max\{0, \alpha(\mathbf{e})\} \leq \min_e \beta(\mathbf{e}) \right\} \supset \mathbf{e}_*, \quad (72)$$

$$\mathcal{E}^* = \bigcup_{j \in J(\mathbf{e})} \left\{ \text{Proj}_e(\mathcal{R}_j) : \beta(\mathbf{e}) \geq \max_e \{\max\{0, \alpha(\mathbf{e})\}\} \right\} \supset \mathbf{e}^*. \quad (73)$$

These expressions result from applying Equations (27-28) to the bounding functions in (69). As before, even though the approach is applicable to any partition of the master domain, tighter bounds are obtained if the partition is finer where either $\bar{g} - \underline{g}$ or $E[\bar{g} - \underline{g}|\mathcal{R}]$ are large.

VI. Global Sensitivity Analysis

In the context of UQ, sampling-based methods⁴ and analysis of variance are widely used sensitivity analysis techniques. These methods evaluate sensitivities by quantifying the contribution of the uncertainty in a particular parameter to the spread in the variance of a performance function. While this information provides some insight as to what parameters are dominant and which ones are not, it fails to account for the effect of such uncertainty in other statistics. Therefore, it is possible that the contribution of the uncertainty in a given parameter to the variance is insignificant, while its contribution to the failure probability is substantial.

In this section we consider the sensitivity of the mean, variance and failure probability to the uncertainty model of \mathbf{p} . The sensitivities are global since they are not restricted to a single

point of the uncertain parameter space, nor to a particular family of distribution functions. If the sensitivity is small, the statistic will not change noticeably when the uncertainty model is changed within the support set, e.g., the UQ of a system where an unimportant parameter is modeled as a random variable supported in Δ is practically identical to the UQ of the system where such a parameter takes any fixed value in Δ . This practice, which can be used to reduce the number of parameters that should be considered uncertain, facilitates the deployment and convergence of UQ methods whose performance, accuracy and correctness is critically linked to the dimension of the parameter space, e.g., polynomial chaos, homothetic deformations, FORM, etc.

For instance, consider the reliability analysis of a system that depends on s independently distributed aleatory variables. Our objective is to determine the sensitivity of the failure probability $P[w(\mathbf{p}) > 0]$ to the uncertainty model of \mathbf{p}_1 . In principle, for each of the infinite number of models that could be chosen to describe \mathbf{p}_1 there is a different value of the failure probability. Note that failure probability range that results from propagating all possible uncertainty models of \mathbf{p}_1 is bounded by the failure probability range corresponding to the subfamily of Dirac deltas. Consequently, we will describe the aleatory variable \mathbf{p}_1 as if it were epistemic. In this setting, the methods of Section V can be used to calculate an outer bounding interval to the failure probability range for $\mathbf{a} = \{\mathbf{p}_2, \dots, \mathbf{p}_s\}$ and $\mathbf{e} = \{\mathbf{p}_1\} \in \Delta_e$. Note that the failure probability corresponding to any uncertainty model of \mathbf{p}_1 supported in Δ_e , -even a probabilistic one- will fall within this interval. Therefore, if the bounding interval is sufficiently small, all uncertainty models of \mathbf{p}_1 supported in Δ_e will lead to practically the same failure probability value. By assuming that \mathbf{p}_1 takes on a fixed, known value in Δ_e without changing the model of $[\mathbf{p}_2, \dots, \mathbf{p}_s]$, we will obtain a failure probability value that differs from any other one we could have obtained by less than the spread of the bounding interval. Therefore, small bounding intervals will indicate the \mathbf{p}_1 can be safely assumed to take on a constant value. If the spread of the bounding interval is large and the partition of Λ near \mathbf{e}_* and \mathbf{e}^* is sufficiently fine, \mathbf{p}_1 is a dominant parameter. In this case the failure probability will be highly sensitive to the uncertainty model of \mathbf{p}_1 .

A mathematical framework supporting these ideas is presented next. Without loss of generality, consider the statistics $E[w]$, $V[w]$ and $R \triangleq P[w > 0] = P[\mathcal{F}]$. Assume that lower and upper bounds to this function, namely $\underline{w}(\mathbf{p})$ and $\overline{w}(\mathbf{p})$, are calculated via Bernstein polynomials. Let L be a set with all the indices of the parameters in \mathbf{p} whose sensitivity is to be determined, while K contains the indices of the remaining aleatory variables. Further assume that the uncertainty model of the variables in L is independent of the uncertainty model of the variables in K . L , which can contain indices of both epistemic and aleatory variables, has m elements where $0 \leq m \leq p - 1$. Denote by Δ_q the support set of $\mathbf{q} = [\mathbf{p}_{L_1}, \dots, \mathbf{p}_{L_m}]$, and by Δ_r the support set of $\mathbf{r} \in \mathbb{R}^{s-m}$.

Our objective is to calculate the sensitivity of the statistics in Equations (6-8), given by

$$E[w; L](\mathbf{q}) = \int_{\Delta_r} w(\mathbf{q}, \mathbf{r}) f_r(\mathbf{r}) d\mathbf{r}, \quad (74)$$

$$R[w; L](\mathbf{q}) = \int_{w(\mathbf{q}, \mathbf{r}) > 0} f_r(\mathbf{r}) d\mathbf{r}, \quad (75)$$

$$V[w; L](\mathbf{q}) = E[w^2; L] - E[w; L]^2, \quad (76)$$

to the uncertainty model of the variables in \mathbf{q} . In this setting, the *global sensitivities* are:

$$\sigma_E(\underline{w}, \bar{w}, L) \triangleq \max_{\mathbf{q} \in \Delta_q} E[\bar{w}; L] - \min_{\mathbf{q} \in \Delta_q} E[\underline{w}; L], \quad (77)$$

$$\sigma_R(\underline{w}, \bar{w}, L) \triangleq \max_{\mathbf{q} \in \Delta_q} R[\bar{w}; L] - \min_{\mathbf{q} \in \Delta_q} R[\underline{w}; L], \quad (78)$$

$$\sigma_V(\underline{w}, \bar{w}, L) \triangleq \max_{\mathbf{q} \in \Delta_q} u[\underline{w}; \bar{w}; L] - \min_{\mathbf{q} \in \Delta_q} l[\underline{w}; \bar{w}; L], \quad (79)$$

where u and l are given by the interval equation

$$[l[\underline{w}; \bar{w}; L], u[\underline{w}; \bar{w}; L]] = E [[\underline{w}, \bar{w}]^2; L] - [E[\underline{w}; L], E[\bar{w}; L]]^2, \quad (80)$$

set according to the developments in Section IV-B. These expressions can be calculated using the developments of Section V by treating \mathbf{q} as if it were an epistemic variable.

If a global sensitivity is ϵ , the corresponding statistic will not change more than ϵ when we chose any uncertainty model for \mathbf{q} supported in Δ_q . When this model is comprised by a collection of Dirac deltas, i.e., when the parameters take on fixed, known values; an accurate reduction in the uncertain parameter dimension is attained. In general, the sensitivities $\sigma_E(\underline{w}, \bar{w}, L)$, $\sigma_R(\underline{w}, \bar{w}, L)$, and $\sigma_V(\underline{w}, \bar{w}, L)$ are, in general, independent of each other; e.g., some parameters may be unimportant according to the failure probability but they may be dominant according to the mean. These following example illustrates these ideas quantitatively.

Example 4: Consider the requirement functions

$$\mathbf{g}_1 = 4\mathbf{p}_1^3 - \mathbf{p}_1^2 + \mathbf{p}_1 - 4\mathbf{p}_1^4 - 400\mathbf{p}_2^2 - 400\mathbf{p}_2^4, \quad (81)$$

$$\mathbf{g}_2 = \frac{1}{5}\mathbf{p}_1^3\mathbf{p}_2^2 + \frac{1}{1000}\mathbf{p}_1^2\mathbf{p}_2^2 - \frac{1}{2}\mathbf{p}_1^3 - \mathbf{p}_1\mathbf{p}_2^2 - \frac{1}{400}\mathbf{p}_1^2 + \frac{5}{2}\mathbf{p}_1 - \frac{5}{2}, \quad (82)$$

defined over the master domain $\mathcal{D} \in [-2, 2] \times [-2, 2]$. Assume that \mathbf{p}_1 is a Beta-distributed random variable with parameters $\langle 7, 7 \rangle$, and \mathbf{p}_2 is a Beta-distributed random variable with parameters $\langle 1, 10 \rangle$ both supported in $[-2, 2]$. We want to determine the global sensitivity of $E[w]$, $V[w]$ and $P[w > 0] = P[\mathbf{g} > \mathbf{0}]$, where w is the worst-case requirement function, to the uncertainty models of \mathbf{p}_1 and \mathbf{p}_2 .

While the sensitivities for the setting $\mathbf{q} = \{\mathbf{p}_1\}$ are $\sigma_E(\underline{w}, \bar{w}, 1) = -2.20391 - (-2.79632) = 0.5924$, $\sigma_V(\underline{w}, \bar{w}, 1) = 1.09538 - 0 = 1.09538$, and $\sigma_R(\underline{w}, \bar{w}, 1) = 0.0042194 - 0 = 0.0042194$; those for $\mathbf{q} = \{\mathbf{p}_2\}$ are $\sigma_E(\underline{w}, \bar{w}, 2) = -0.56841 - (-2.57057) = 2.0022$, $\sigma_V(\underline{w}, \bar{w}, 2) = 2.86507 - 0 = 2.86507$, and $\sigma_R(\underline{w}, \bar{w}, 2) = 0.47571 - 0 = 0.47571$. Figure 12 shows the bounds on the mean and variance functions from where the sensitivities were calculated. The largest and smallest values of the bounding functions determine σ_E and σ_V . While the sensitivity of the failure probability to uncertainty in \mathbf{p}_2 is 112 times larger than that for \mathbf{p}_1 , the sensitivity of the mean to uncertainty in \mathbf{p}_2 is 3.38 times larger than that for \mathbf{p}_1 . If a failure probability of less than 0.0042194 is acceptable, \mathbf{p}_1 can be assumed to take on any constant value in $[-2, 2]$.

In this example, estimates of the functions $E[w(\mathbf{q})]$ and $V[w(\mathbf{q})]$ can be readily calculated using Monte Carlo sampling. These functions will fall between the bounds shown in Figure 12. The extrema of such functions, which can be calculated via optimization, can be used

to approximate the global sensitivities above. This practice will render meaningful values as long as the optimizer has converged to the global extrema. Unfortunately, the moments of piecewise polynomial functions may not only have derivative discontinuities but also multiple local extrema. In contrast to this practice, the approach proposed yields results whose correctness is formally verifiable.

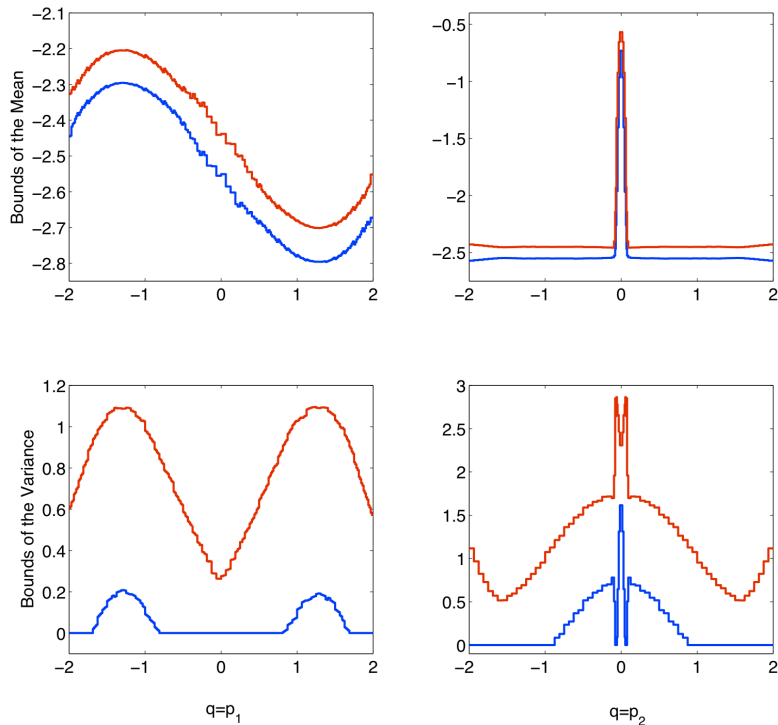


Figure 12. Mean (top) and variance (bottom) bounds for $q = \{p_1\}$ (left) and $q = \{p_2\}$ (right).

VII. Conclusions

This paper presents an uncertainty quantification framework that enables the rigorous analysis of polynomial systems subject to both aleatory and epistemic uncertainties. The Bernstein expansion approach enables the calculation of analytical bounds to moments and failures probabilities as well as finding supersets of the corresponding best- and worst-case epistemic realizations. These bounds and supersets can be made as tight and as small as desired. Furthermore, the framework enables determining the importance of particular uncertain parameters according to the manner in which they affect the failure probability, the mean and the variance of a response metric. This information enables ranking the uncertain parameters according to the sensitivity of these three statistics. By modelling inconsequential parameters as deterministic quantities, the size of the uncertain parameter space can be reduced without incurring in significant error. The method proposed generates bounds to this error. The analytical nature of the approach eliminates the numerical error that characterizes the sampling-based techniques commonly used to propagate aleatory uncertainties as well

as the possibility of under predicting the range of the statistic of interest that may result from searching for the best- and worst-case epistemic values via nonlinear optimization or sampling.

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