

## COMPUTATION OF FAILURE PROBABILITY SUBJECT TO EPISTEMIC UNCERTAINTY\*

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**Abstract.** Computing failure probability is a fundamental task in many important practical problems. The computation, its numerical challenges aside, naturally requires knowledge of the probability distribution of the underlying random inputs. On the other hand, for many complex systems it is often not possible to have complete information about the probability distributions. In such cases the uncertainty is often referred to as epistemic uncertainty, and straightforward computation of the failure probability is not available. In this paper we develop a method to estimate both the upper bound and the lower bound of the failure probability subject to epistemic uncertainty. The bounds are rigorously derived using the variational formulas for relative entropy. We examine in detail the properties of the bounds and present numerical algorithms to efficiently compute them.

**Key words.** failure probability, uncertainty quantification, epistemic uncertainty, relative entropy

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**1. Introduction.** Probability of failure is an important quantity in many applications involving system safety, risk management, reliability analysis, etc. Accurate computation of failure probability is thus of fundamental significance. A large amount of literature has been devoted to this task, ranging from more mathematically rigorous studies for model problems to more heuristic ones for engineering systems.

This paper seeks to study the problem in a different context. That is, we study how to estimate the probability of failure when complete knowledge of the input probability distribution is not available. When lack of knowledge is the primary source of the uncertainty, it is often referred to as *epistemic uncertainty*. Though different definitions and classifications exist in the literature, in this paper we will use epistemic uncertainty to refer to the random inputs whose complete information about the probability distribution is not available and use *aleatory uncertainty* to refer to the random inputs whose probability distribution is fully prescribed.

The study of the impacts of epistemic uncertainty is more difficult because many of the existing probabilistic tools do not readily apply. Some of the existing approaches include evidence theory [7], possibility theory [3], and interval analysis [6, 12]. These methods have their own advantages, though most do not address efficient numerical implementations. More recent studies employ approximation theory [1, 5, 13, 8].

This paper is largely motivated by the work of [2], where a method utilizing the variational formulas of relative entropy is developed to derive upper bounds for the predictions of epistemic uncertainty computations. In this paper we develop a methodology, similar to that of [2], for failure probability computation. Most notably we derive *both the upper bound and the lower bound* for the failure probability subject

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to epistemic inputs. The bounds are rigorous and tight—there are no constant factors. In addition to the mathematical derivations, we also discuss numerical algorithms to effectively compute these bounds. The bounds can be highly useful in practical problems, in the sense that one will have good estimates of both the “best-case scenario” and the “worst-case scenario” for the probability of failure. It is worth noting that a similar problem has been studied in [11], where both the probability distribution function and the function defining failure can be unknown. This is a broader setup and is tackled by using concentration-of-measure inequalities. It results in an optimization problem in infinite dimensions and is one of the focuses of [11]. Here we focus on the problem with only unknown probability distribution functions. Our approach utilizes variational inequalities of relative entropy and results in an optimization problem of a single real parameter. The existence of the supremum and infimum of the optimization problem is established; hence the optimization problem can be solved easily.

This paper is organized as follows. After setting up the problem and notation in section 2, we derive both the lower bound and the upper bound in section 3. The estimates are then extended to the case of mixed-type random inputs with both epistemic and aleatory uncertainty in section 4. Numerical algorithms for computing the bounds are briefly discussed in section 5. We then provide numerical examples in section 6 to illustrate the properties of the bounds, before concluding the paper in section 7.

**2. Problem setup.** Throughout this paper we adopt the standard notation  $(\Omega, \mathcal{F}, \mathcal{P})$  to denote a probability space, where  $\Omega$  is the event space,  $\mathcal{F}$  the  $\sigma$ -algebra, and  $\mathcal{P}$  the probability measure, and denote by  $\mathcal{P}(\Omega)$  the set of probability measures on  $(\Omega, \mathcal{F})$ . Let  $y = (y_1, y_2, \dots, y_{n_y})$  be an  $n_y$ -dimensional ( $n_y \geq 1$ ) random variable with distribution function  $\rho(y)$ . The failure probability,  $P_f$ , is a multidimensional integral defined as follows:

$$(2.1) \quad P_f = \text{Prob}(y \in \Omega_f) = \int \mathbb{I}_{\Omega_f} \rho(dy),$$

where  $\mathbb{I}$  is the characteristic function satisfying

$$\mathbb{I}_{\Omega_f}(y) = \begin{cases} 1, & y \in \Omega_f, \\ 0, & y \notin \Omega_f, \end{cases}$$

and  $\Omega_f$  is the failure region defined as

$$(2.2) \quad \Omega_f = \{y : g(y) < 0\}.$$

Here the function  $g$  is the *limit state function*, or *failure function*, that determines when failure occurs. Note that in most practical systems the random variable  $y$  represents the various kinds of uncertain inputs to a complex system, and the function  $g$  represents a complicated mapping between the input uncertainty  $y$  and the output quantity of interest that defines failure. For example, in a structural design problem,  $y$  may represent the uncertainty in the system parameters, constitutive laws, boundary and initial conditions, external forcing, etc., and the failure function may be defined as  $g(y) = \text{strength}(y) - \text{load}(y)$ , with  $g < 0$  representing the failure of the system. The explicit form of  $g$  is not known for most systems and can only be simulated numerically or tested experimentally in a sampling manner. Since most of the practical systems are highly complex and time-consuming to simulate, accurate computation of failure probability is a challenging task.

There exist a large variety of methods for failure probability computation. Roughly speaking, the methods fall into two categories, sampling-based methods and nonsampling-based methods, where the former are mostly originated from Monte Carlo sampling (MCS) and the latter utilize techniques such as response surface/surrogate or asymptotic approximation such as first-order reliability analysis. We will not engage in an extensive review of these methods, because in this paper we will study the problem in a different context—epistemic uncertainty.

**2.1. Epistemic uncertainty.** The calculation of failure probability (2.1) depends obviously on the probability measure  $\rho$ . In almost all the existing methods for failure probability computation, it is assumed that the probability measure is known. However, in practice this information is rarely available. Due to our lack of knowledge of the large variety of input uncertainty, it is very difficult, if not impossible, to fully specify the probability distribution of all the uncertain inputs. In the literature this is often referred to as *epistemic uncertainty*. While it is due to our lack of knowledge, uncertainty of statistical nature with full probabilistic information is often referred to as *aleatory uncertainty*. Here we refrain from more engaging discussions on the categorization of uncertainty, as it is beyond the scope of this paper.

The epistemic uncertainty considered in this paper is defined as follows: (1) it is of parametric type, i.e., it stems from uncertainty in the physical parameters of a system and/or in the hyperparameters characterizing the random inputs of the system (e.g., random variables in Karhunen–Loève expansion of certain input random processes) and (2) its complete probability distribution is unavailable. Some possible scenarios are as follows: (i) The distribution of a parameter is unknown and there is no sufficient information/measurement to suggest it is Gaussian, uniform, or anything else. (ii) The distribution of a parameter is known only to a certain degree. For example, there is enough evidence to suggest that a parameter has a Gaussian distribution. However, its mean and/or variance cannot be specified precisely due to lack of measurement. (iii) The marginal distributions of a set of parameters are known, but the joint distributions among them are not known. Note that this is pervasive in most problems with multiple uncertain parameters, particularly for non-Gaussian distributions. And certainly one can conjure up many more similar situations. Uncertainty quantification in this context thus presents a different challenge, for most of the existing probabilistic tools are not readily applicable because of the lack of probability information.

In this paper we confine ourselves to the problem of (2.1) and focus on how to obtain a reliable estimate of  $P_f$  when the underlying probability measure  $\rho$  is not known.

**3. Bound estimation for epistemic uncertainty.** In this section we establish both the lower bound and the upper bound for the failure probability estimation (2.1). The results are stated using generic notation of  $\gamma$  and  $\rho$  for probability measures.

**3.1. Relative entropy.** As a measurement of the difference between two probability measures, *relative entropy* plays an important role. Once again let  $(\Omega, \mathcal{F}, \mathcal{P})$  be a probability space and  $\mathcal{P}(\Omega)$  be the set of probability measures on  $(\Omega, \mathcal{F})$ . For  $\rho \in \mathcal{P}(\Omega)$ , the *relative entropy*, or the *cross entropy*,  $R(\cdot\|\rho) : \mathcal{P}(\Omega) \rightarrow \mathbb{R} \cup \{\infty\}$  is defined as

$$(3.1) \quad R(\gamma\|\rho) \triangleq \int_{\Omega} \log \left( \frac{d\gamma}{d\rho} \right) d\gamma$$

whenever  $\gamma$  is absolutely continuous with respect to  $\rho$ ; otherwise, we set  $R(\gamma\|\rho) \triangleq \infty$ . Among the many properties of the relative entropy, we here introduce the following ones that are relevant in our paper.

LEMMA 3.1. *Let  $\gamma, \rho \in \mathcal{P}(\Omega)$ . Then*

- (a)  $R(\gamma\|\rho) \geq 0$  and  $R(\gamma\|\rho) = 0$  if and only if  $\gamma = \rho$ ;
- (b) if  $\gamma$  is absolutely continuous with respect to  $\rho$ , then  $R(\gamma\|\rho) < \infty$ .

For other properties such as  $R(\cdot\|\cdot)$  being a convex, lower semicontinuous function with compact level sets, etc., readers are referred to [4].

**3.2. Lower bound.** An important property of the relative entropy is a variational duality between the exponential integral and the relative entropy. This is the basis for our derivation of the lower bound for (2.1). Here we restate Proposition 1.4.2 in [4] and leave its details and proof to [4].

PROPOSITION 3.2 ([4]). *Let  $(\Omega, \mathcal{F}, \mathcal{P})$  be a probability space,  $k$  be a bounded measurable function mapping  $\Omega$  into  $\mathbb{R}$ , and  $\rho \in \mathcal{P}(\Omega)$ . Then the following conclusions hold:*

$$(a) \quad (3.2) \quad -\log \int_{\Omega} e^{-k} d\rho = \inf_{\gamma \in \mathcal{P}(\Omega)} \left[ R(\gamma\|\rho) + \int_{\Omega} k d\gamma \right].$$

- (b) Let  $\gamma_0 \in \mathcal{P}(\Omega)$  be absolutely continuous with respect to  $\rho$  and satisfy

$$(3.3) \quad \frac{d\gamma_0}{d\rho}(x) \triangleq \frac{e^{-k(x)}}{\int_{\Omega} e^{-k} d\rho}.$$

Then the infimum in the variational formula (3.2) is uniquely attained at  $\gamma_0$ .

A straightforward conclusion from Proposition 3.2 can be presented as follows.

COROLLARY 3.3. *Under the same assumptions as in Proposition 3.2, one has*

$$(3.4) \quad \int_{\Omega} k d\gamma \geq -\log \int_{\Omega} e^{-k} d\rho - R(\gamma\|\rho) \quad \text{for any } \gamma \in \mathcal{P}(\Omega).$$

Since the characteristic function  $\mathbb{I}_{\Omega_f}$  in (2.1) is naturally bounded and measurable, we set the function  $k$  in (3.2) to be  $c\mathbb{I}_{\Omega_f}$ ,  $c > 0$ , and immediately obtain the following result.

COROLLARY 3.4. *For any  $\rho \in \mathcal{P}(\Omega)$ ,*

$$(3.5) \quad -\log \int_{\Omega} e^{-c\mathbb{I}_{\Omega_f}} d\rho = \inf_{\gamma \in \mathcal{P}(\Omega)} \left[ R(\gamma\|\rho) + \int_{\Omega} c\mathbb{I}_{\Omega_f} d\gamma \right] \quad \text{for any } c \in (0, \infty).$$

It follows that

$$(3.6) \quad \int_{\Omega} \mathbb{I}_{\Omega_f} d\gamma \geq -\frac{1}{c} \log \int_{\Omega} e^{-c\mathbb{I}_{\Omega_f}} d\rho - \frac{1}{c} R(\gamma\|\rho) \quad \text{for any } \gamma \in \mathcal{P}(\Omega).$$

As a result, we obtain a *lower bound* of the failure probability (2.1) using an arbitrary probability measure  $\gamma$ :

$$(3.7) \quad \int_{\Omega} \mathbb{I}_{\Omega_f} d\gamma \geq \sup_{c \in (0, \infty)} \left[ -\frac{1}{c} \log \int_{\Omega} e^{-c\mathbb{I}_{\Omega_f}} d\rho - \frac{1}{c} R(\gamma\|\rho) \right] \quad \text{for any } \gamma \in \mathcal{P}(\Omega).$$

**3.3. Upper bound.** To obtain the upper bound of the failure probability estimate using a different probability measure, we state Lemma 1.4.3(a) in [4].

LEMMA 3.5 (Donsker–Varadhan variational formula). *Let  $\mathcal{C}_b(\Omega)$  be the space of bounded continuous functions mapping  $\Omega$  into  $\mathbb{R}$  and  $\Psi_b(\Omega)$  be the space of bounded Borel-measurable functions mapping  $\Omega$  into  $\mathbb{R}$ . Then for  $\gamma, \rho \in \mathcal{P}(\Omega)$ ,*

$$(3.8) \quad R(\gamma\|\rho) = \sup_{g \in \mathcal{C}_b(\Omega)} \left[ \int_{\Omega} g d\gamma - \log \int_{\Omega} e^g d\rho \right] = \sup_{\psi \in \Psi_b(\Omega)} \left[ \int_{\Omega} \psi d\gamma - \log \int_{\Omega} e^{\psi} d\rho \right].$$

It then follows that for any  $\psi \in \Psi_b(\Omega)$ ,

$$(3.9) \quad \int_{\Omega} \psi d\gamma \leq R(\gamma\|\rho) + \log \int_{\Omega} e^{\psi} d\rho.$$

For the failure probability problem (2.1), we let  $\psi = c\mathbb{I}_{\Omega_f}$ , where  $c \in (0, \infty)$ , and obtain

$$(3.10) \quad \int_{\Omega} \mathbb{I}_{\Omega_f} d\gamma \leq \frac{1}{c} R(\gamma\|\rho) + \frac{1}{c} \log \int_{\Omega} e^{c\mathbb{I}_{\Omega_f}} d\rho.$$

An upper bound immediately follows as

$$(3.11) \quad \int_{\Omega} \mathbb{I}_{\Omega_f} d\gamma \leq \inf_{c \in (0, \infty)} \left[ \frac{1}{c} R(\gamma\|\rho) + \frac{1}{c} \log \int_{\Omega} e^{c\mathbb{I}_{\Omega_f}} d\rho \right].$$

**3.4. Properties of the bounds.** For notational convenience, we employ the following definitions for the exponential integrals. For any  $c > 0$ , let

$$(3.12) \quad \begin{aligned} \Theta^-(c) &\triangleq -\frac{1}{c} \log \int_{\Omega} e^{-c\mathbb{I}_{\Omega_f}} d\rho, \\ \Theta^+(c) &\triangleq \frac{1}{c} \log \int_{\Omega} e^{c\mathbb{I}_{\Omega_f}} d\rho. \end{aligned}$$

Note that by l'Hôpital's rule, we immediately have

$$(3.13) \quad \begin{aligned} \lim_{c \rightarrow 0^+} \Theta^-(c) &= \int_{\Omega} \mathbb{I}_{\Omega_f} d\rho, \\ \lim_{c \rightarrow 0^+} \Theta^+(c) &= \int_{\Omega} \mathbb{I}_{\Omega_f} d\rho. \end{aligned}$$

These naturally allow us to extend the definitions for  $\Theta^-(c)$  and  $\Theta^+(c)$  to  $c \in [0, \infty)$ .

We now summarize the established results of the upper bound (3.11) and lower bound (3.7) into the following statement.

THEOREM 3.6. *Let  $(\Omega, \mathcal{F}, \mathcal{P})$  be a probability space and  $\rho \in \mathcal{P}(\Omega)$  be a measure, and define*

$$(3.14) \quad R^* = \sup_{\gamma \in \mathcal{A}} R(\gamma\|\rho),$$

where  $\mathcal{A} \subseteq \mathcal{P}(\Omega)$  is a set of probability measures. With the definitions of  $\Theta^+$  and  $\Theta^-$  in (3.12), define

$$(3.15) \quad P_f^u \triangleq \inf_{c \in (0, \infty)} \left[ \Theta^+(c) + \frac{1}{c} R^* \right]$$

and

$$(3.16) \quad P_f^\ell \triangleq \sup_{c \in (0, \infty)} \left[ \Theta^-(c) - \frac{1}{c} R^* \right].$$

Then, the failure probability integral (2.1) satisfies

$$(3.17) \quad P_f^\ell \leq \int \mathbb{I}_{\Omega_f} d\gamma \leq P_f^u \quad \text{for any } \gamma \in \mathcal{A}.$$

Important properties of the upper bound involving  $\Theta^+$  have been established in [2]. Here we generalize the properties to the lower bound involving  $\Theta^-$ .

**PROPOSITION 3.7.** *Let  $D = \{c : \Theta^+(c) < \infty\}$  and  $E = \{c : \Theta^-(c) > -\infty\}$ , where  $\Theta^+$  and  $\Theta^-$  are defined in (3.12). Denote by  $D^\circ$  the interior of  $D$  and  $E^\circ$  the interior of  $E$ , and assume  $D^\circ \neq \emptyset$  and  $E^\circ \neq \emptyset$ . Let  $R^*$  be a positive constant. Then the following conclusions hold:*

- (a)  $\Theta^+(c)$  is differentiable on  $D^\circ$  and nondecreasing for  $c \geq 0$ . There is a unique  $c \in (0, \infty]$  at which  $\Theta^+(c) + \frac{1}{c} R^*$  attains a local minimum. The minimum occurring at  $c = \infty$  means that  $\Theta^+(c) + \frac{1}{c} R^* > \lim_{c \rightarrow \infty} \Theta^+(c)$  for a well-defined  $\lim_{c \rightarrow \infty} \Theta^+(c)$ .
- (b)  $\Theta^-(c)$  is differentiable on  $E^\circ$  and nonincreasing for  $c \geq 0$ . There exists a unique  $c \in (0, \infty]$  at which  $\Theta^-(c) - \frac{1}{c} R^*$  achieves a local maximum. The maximum occurring at  $c = \infty$  means that  $\Theta^-(c) - \frac{1}{c} R^* < \lim_{c \rightarrow \infty} \Theta^-(c)$  for a well-defined  $\lim_{c \rightarrow \infty} \Theta^-(c)$ .

*Proof.* Part (a) is a direct consequence of Proposition 3 in [2], by using the fact that  $\mathbb{I}_{\Omega_f}$  is bounded and positive. We will leave the details of the proof to [2].

For part (b), let  $H(c) \triangleq c \cdot \Theta^-(c) = -\log \int e^{-c\mathbb{I}_{\Omega_f}} \rho(dx)$ . Then  $0 \leq H(c) \leq 1$  for any  $c \geq 0$  and  $H(0) = 0$ . Consider

$$H'(c) = \frac{\int \mathbb{I}_{\Omega_f} e^{-c\mathbb{I}_{\Omega_f}} \rho(dx)}{\int e^{-c\mathbb{I}_{\Omega_f}} \rho(dx)}$$

and

$$\begin{aligned} H''(c) &= \left( \frac{\int \mathbb{I}_{\Omega_f} e^{-c\mathbb{I}_{\Omega_f}} \rho(dx)}{\int e^{-c\mathbb{I}_{\Omega_f}} \rho(dx)} \right)^2 - \frac{\int \mathbb{I}_{\Omega_f}^2 e^{-c\mathbb{I}_{\Omega_f}} \rho(dx)}{\int e^{-c\mathbb{I}_{\Omega_f}} \rho(dx)} \\ &= (H'(c))^2 - H'(c). \end{aligned}$$

Since  $0 \leq \mathbb{I}_{\Omega_f} \leq 1$ , it follows that  $0 \leq H'(c) \leq 1$ ; then  $H''(c) \leq 0$ . As a result,  $H(c)$  is a nondecreasing and concave function and  $H'(c)$  is nonincreasing. The fact that

$$(3.18) \quad \frac{1}{c} H(c) = \frac{1}{c} (H(c) - H(0)) = \frac{1}{c} \int_0^c H'(t) dt$$

implies  $\Theta^-(c) = \frac{1}{c} H(c)$  is nonincreasing for  $c \geq 0$ .

To establish the local unique maximum, let us first assume  $M \triangleq \sup E = \infty$ . Taking the derivative of  $\Theta^-(c) - \frac{1}{c} R^*$  then gives

$$\frac{d}{dc} \left[ \frac{1}{c} H(c) - \frac{1}{c} R^* \right] = \frac{1}{c^2} [cH'(c) - H(c) + R^*].$$

Define a mapping  $f : [0, \infty) \rightarrow \mathbb{R}$  as  $f(c) = cH'(c) - H(c)$ ; then  $f(0) = 0$ . Observing that  $f'(c) = cH''(c) \leq 0$ , then  $f(c)$  is monotonically decreasing on  $[0, \infty)$ . If  $\lim_{c \rightarrow \infty} f(c) < -R^*$ , then there is a unique solution to  $cH'(c) - H(c) + R^* = 0$  and the claim is satisfied. If  $\lim_{c \rightarrow \infty} f(c) \geq -R^*$ , then  $\frac{1}{c}H(c) - \frac{1}{c}R^*$  is monotonically increasing on  $[0, \infty)$ . It follows from (3.18) that  $\frac{1}{c}H(c) \leq H'(0) \leq 1$ , as  $H'(c)$  is nonincreasing for  $c \in [0, \infty)$ . Then there exists a well-defined limit  $\lim_{c \rightarrow \infty} \frac{1}{c}H(c) = \lim_{c \rightarrow \infty} [\frac{1}{c}H(c) - \frac{1}{c}R^*]$ , which is the required maximum.

Next let us consider the case of  $M \in (0, \infty)$ . It is straightforward to see that  $H(c) \uparrow \infty$  and  $H'(c) \downarrow -\infty$  as  $c \uparrow M$  because of the monotonic convergence. Let  $0 < b < c < M$ ; then the relation

$$H(c) = \int_0^c H'(t)dt \geq bH'(b) + (c-b)H'(c)$$

implies  $cH'(c) - H(c) \leq b(H'(c) - H'(b))$ . By fixing  $b$  and letting  $c \uparrow M$ , it follows that  $cH'(c) - H(c) \downarrow -\infty$  as  $c \uparrow M$ . By applying the same argument in the case of  $M = \infty$ , the conclusion can be established.  $\square$

A direct consequence of Proposition 3.7 is that the minimum of the upper bound and the maximum of the lower bound in Theorem 3.6 exist and can be computed by a particular optimization algorithm.

**3.5. Short summary and remarks.** Here we collect the above results into a short summary and provide an itemized algorithm to illustrate the implementation of the results. For a practical problem where the probability function of the input variables are unknown, the procedure for computing the bounds on the failure probability is as follows:

- (1) Identify a set of probability measures  $\mathcal{A} \subseteq \mathbb{P}(\Omega)$ . In practice, this set corresponds to the possible/allowable probability distributions that the uncertain inputs may possess.
- (2) Choose a nominal probability measure  $\rho$ . In principle, this nominal probability can be arbitrary. However, it is desirable to choose  $\rho$  to be in the set  $\mathcal{A}$  based on the best available information about the probability distribution of the inputs.
- (3) Compute  $R^*$  by (3.14). This step is usually carried out analytically or with negligible numerical error.
- (4) Compute both the upper bound and the lower bound using Theorem 3.6 via the optimization problems (3.15) and (3.16). Here the quantities  $\Theta^-(c)$  and  $\Theta^+(c)$  are defined in (3.12).

We remark that the computation of  $\Theta^-(c)$  and  $\Theta^+(c)$  using (3.12) involves evaluating integrals in the failure domain. It requires simulation or experimentation of the underlying stochastic system and can be expensive. However, this kind of forward stochastic problem is pervasive in most stochastic problems, and it is reasonable to conduct at least one set of forward problem computations. The optimization problems (3.15) and (3.16), however, do not add more simulation cost, as the same samples can be used for all values of  $c$ . This will become clearer in section 5 when numerical methods are discussed.

We also remark that the “allowable” set  $\mathcal{A}$  of probability measures should be chosen as small as possible, using the best available information, to obtain tight bounds. From a mathematical point of view, the set  $\mathcal{A}$  can be arbitrarily large. However, the larger the set  $\mathcal{A}$  is, the wider the bounds of the failure probability

will be. This is a natural reflection of less available information about the inputs, regardless of the technique one utilizes to estimate the bounds.

**4. Bound estimation for mixed aleatory and epistemic uncertainty.** We now generalize the above results to the case of mixed aleatory and epistemic uncertainty. From this point on we will reserve the variable  $x$  for the aleatory variable with known probability measure  $\mu(x)$  and the variable  $y$  for the epistemic variable whose probability distribution is not completely known. We also denote the domain of the aleatory variable  $x$  as  $\Omega_1$  and that of the epistemic variable  $y$  as  $\Omega_2$ . Obviously,  $\Omega_1 \otimes \Omega_2 = \Omega$  and  $(\Omega_1, \mathcal{F}_1, \mathcal{P}(\Omega_1))$  and  $(\Omega_2, \mathcal{F}_2, \mathcal{P}(\Omega_2))$  are probability spaces. The failure probability  $P_f$  in (2.1) is then rewritten as

$$(4.1) \quad \tilde{P}_f = \int_{\Omega_2} \int_{\Omega_1} \mathbb{I}_{\Omega_f}(x, y) \mu(dx) \rho(dy),$$

where  $\mu$  is known and  $\rho$  is unknown.

We employ a similar technique as in [2] and generalize the definitions (3.12) to the case of mixed-form uncertainty. Two forms of generalizations can be constructed. The first form is a straightforward separation of the aleatory and epistemic variables in the exponential integral. That is, for  $c > 0$ , let

$$(4.2) \quad \begin{aligned} \Lambda^+(c) &\triangleq \frac{1}{c} \log \int_{\Omega_2} \int_{\Omega_1} e^{c\mathbb{I}_{\Omega_f}(x, y)} \mu(dx) \rho(dy), \\ \Lambda^-(c) &\triangleq -\frac{1}{c} \log \int_{\Omega_2} \int_{\Omega_1} e^{-c\mathbb{I}_{\Omega_f}(x, y)} \mu(dx) \rho(dy). \end{aligned}$$

The second form of generalization integrates the aleatory variable in the exponential function first and takes the following form, for  $c > 0$ :

$$(4.3) \quad \begin{aligned} \Lambda_1^+(c) &\triangleq \frac{1}{c} \log \int_{\Omega_2} e^{\int_{\Omega_1} c\mathbb{I}_{\Omega_f}(x, y) \mu(dx)} \rho(dy), \\ \Lambda_1^-(c) &\triangleq -\frac{1}{c} \log \int_{\Omega_2} e^{\int_{\Omega_1} -c\mathbb{I}_{\Omega_f}(x, y) \mu(dx)} \rho(dy). \end{aligned}$$

Since the limits of these quantities are well defined,

$$\lim_{c \rightarrow 0^+} \Lambda^-(c), \Lambda_1^-(c), \Lambda^+(c), \Lambda_1^+(c) = \int_{\Omega_2} \int_{\Omega_1} \mathbb{I}_{\Omega_f}(x, y) \mu(dx) \rho(dy),$$

their definitions can be easily extended onto  $[0, \infty)$  by setting  $\Lambda^-(0), \Lambda^+(0), \Lambda_1^-(0)$ , and  $\Lambda_1^+(0)$  to be the aforementioned limit.

Upon applying Jensen's inequality to the exponential function, we obtain  $\Lambda_1^+(c) < \Lambda^+(c)$  and  $\Lambda_1^-(c) > \Lambda^-(c)$ . By setting  $\psi = \int_{\Omega_1} c\mathbb{I}_{\Omega_f} \mu(dx)$ ,  $c > 0$ , in (3.9), we obtain the following inequality:

$$(4.4) \quad \int_{\Omega_2} \int_{\Omega_1} \mathbb{I}_{\Omega_f}(x, y) \mu(dx) \rho(dy) \leq \frac{1}{c} R(\rho(dy) \| \gamma(dy)) + \Lambda_1^+(c) \quad \text{for any } \gamma \in \mathcal{P}(\Omega_2),$$

where  $R(\rho \| \gamma)$  is the relative entropy between measures  $\rho$  and  $\gamma$ , defined in (3.1). Similarly, by setting  $k = \int_{\Omega_1} c\mathbb{I}_{\Omega_f} \mu(dx)$ ,  $c > 0$ , in (3.4), we obtain

$$(4.5) \quad \int_{\Omega_2} \int_{\Omega_1} \mathbb{I}_{\Omega_f}(x, y) \mu(dx) \rho(dy) \geq -\frac{1}{c} R(\rho(dy) \| \gamma(dy)) + \Lambda_1^-(c) \quad \text{for any } \gamma \in \mathcal{P}(\Omega_2).$$

Since  $c$  is an arbitrary positive constant, (4.4) and (4.5) immediately result in an upper bound and a lower bound for the failure probability (4.1), summarized in the following statement.

**THEOREM 4.1.** *Let  $(\Omega_1, \mathcal{F}_1, \mathcal{P}(\Omega_1))$  and  $(\Omega_2, \mathcal{F}_2, \mathcal{P}(\Omega_2))$  be the probability spaces as defined above. Let  $\mu \in \mathcal{P}(\Omega_1)$  and  $\rho \in \mathcal{P}(\Omega_2)$  and define*

$$(4.6) \quad R^* = \sup_{\gamma \in \mathcal{A}} R(\gamma(dy) \parallel \rho(dy)),$$

where  $\mathcal{A} \subseteq \mathcal{P}(\Omega_2)$  is a set of probability measures. With the definitions of  $\Lambda_1^+$  and  $\Lambda_1^-$  in (4.3), define

$$(4.7) \quad \begin{aligned} \tilde{P}_f^u &\triangleq \inf_{c \in (0, \infty)} \left[ \frac{1}{c} R(\rho(dy) \parallel \gamma(dy)) + \Lambda_1^+(c) \right], \\ \tilde{P}_f^\ell &\triangleq \sup_{c \in (0, \infty)} \left[ -\frac{1}{c} R(\rho(dy) \parallel \gamma(dy)) + \Lambda_1^-(c) \right]. \end{aligned}$$

Then, the failure probability integral (4.1) satisfies

$$(4.8) \quad \tilde{P}_f^u \leq \int_{\Omega_2} \int_{\Omega_1} \mathbb{I}_{\Omega_f}(x, y) \mu(dx) \gamma(dy) \leq \tilde{P}_f^\ell \quad \text{for any } \gamma \in \mathcal{A}.$$

Similar to the epistemic uncertainty case, statements regarding the minimum and maximum of the failure probability can be made.

**PROPOSITION 4.2.** *Let  $D = \{c : \Lambda_1^+(c) < \infty\}$  and  $E = \{c : \Lambda_1^-(c) > -\infty\}$ , where  $\Lambda_1^+$  and  $\Lambda_1^-$  are defined in (4.2). Denote  $D^\circ$  as the interior of  $D$  and  $E^\circ$  as the interior of  $E$  and assume  $D^\circ \neq \emptyset$  and  $E^\circ \neq \emptyset$ . Let  $R^*$  be a positive constant. Then the following conclusions hold:*

- (a)  $\Lambda_1^+(c)$  is differentiable on  $D^\circ$  and nondecreasing for  $c \geq 0$ . There is a unique  $c \in (0, \infty]$  at which  $\Lambda_1^+(c) + \frac{1}{c}R^*$  attains a local minimum. The minimum occurring at  $c = \infty$  means that  $\Lambda_1^+(c) + \frac{1}{c}R^* > \lim_{c \rightarrow \infty} \Lambda_1^+(c)$  for a well-defined  $\lim_{c \rightarrow \infty} \Lambda_1^+(c)$ .
- (b)  $\Lambda_1^-(c)$  is differentiable on  $E^\circ$  and nonincreasing for  $c \geq 0$ . There exists a unique  $c \in (0, \infty]$  at which  $\Lambda_1^-(c) - \frac{1}{c}R^*$  achieves a local maximum. The maximum occurring at  $c = \infty$  means that  $\Lambda_1^-(c) - \frac{1}{c}R^* < \lim_{c \rightarrow \infty} \Lambda_1^-(c)$  for a well-defined  $\lim_{c \rightarrow \infty} \Lambda_1^-(c)$ .

*Proof.* Part (a) is a direct consequence of Proposition 3 in [2] by setting the nonnegative function  $F$  there to be  $F(y) = \int_{\Omega_1} \mathbb{I}_{\Omega_f} \mu(dx)$ .

For part (b), let us define

$$H(c) \triangleq c \cdot \Lambda_1^-(c) = -\log \int_{\Omega_2} e^{-c \int_{\Omega_1} \mathbb{I}_{\Omega_f} \mu(dx)} \rho(dy).$$

It follows immediately that  $0 \leq H(c) \leq 1$ ,  $H(0) = 0$ ,  $0 \leq H'(c) \leq 1$ , and  $H''(c) \leq 0$ . With these preparations and by following the same steps as in the proof of Proposition 3.7(b), we establish the claim here.  $\square$

By exploring the behavior of the hybrid forms  $\Lambda_1^+(c)$  and  $\Lambda_1^-(c)$  when  $c$  goes to  $\infty$ , we obtain the following result.

**THEOREM 4.3.** *With all assumptions stated as before and  $\Lambda_1^+$  and  $\Lambda_1^-$  defined in (4.3), assume  $\Omega_1$  and  $\Omega_2$  are finite-dimensional spaces. Then the following relations hold:*

$$(4.9) \quad \begin{aligned} \operatorname{ess\,sup}_{y \in \Omega_2} \int_{\Omega_1} \mathbb{I}_{\Omega_f}(x, y) \mu(dx) &= \lim_{c \rightarrow \infty} \Lambda_1^+(c), \\ \operatorname{ess\,inf}_{y \in \Omega_2} \int_{\Omega_1} \mathbb{I}_{\Omega_f}(x, y) \mu(dx) &= \lim_{c \rightarrow \infty} \Lambda_1^-(c). \end{aligned}$$

*Proof.* For notational convenience, let us define

$$(4.10) \quad V(y) = \int_{\Omega_1} \mathbb{I}_{\Omega_f}(x, y) \mu(dx),$$

which is the volume of the failure domain projected on the  $y$ -plane. Naturally  $V(y)$  is bounded and nonnegative for any  $y \in \Omega_2$ . Then,

$$(4.11) \quad \begin{aligned} \Lambda_1^+(c) &= \frac{1}{c} \log \int_{\Omega_2} e^{cV(y)} \rho(dy) \\ &= \log \left( \int_{\Omega_2} e^{cV(y)} \rho(dy) \right)^{\frac{1}{c}} \\ &= \log \|e^{V(y)}\|_{L_c(\Omega_2)}. \end{aligned}$$

As a result,

$$(4.12) \quad \begin{aligned} \lim_{c \rightarrow \infty} \Lambda_1^+(c) &= \log \|e^{V(y)}\|_{\infty} \\ &= \log(e^{\|V(y)\|_{\infty}}) \\ &= \operatorname{ess\,sup}_{y \in \Omega_2} V(y). \end{aligned}$$

Similarly, for  $\Lambda_1^-(c)$ , we have

$$(4.13) \quad \begin{aligned} \Lambda_1^-(c) &= -\frac{1}{c} \log \int_{\Omega_2} e^{-cV(y)} \rho(dy) \\ &= -\log \left( \int_{\Omega_2} e^{-cV(y)} \rho(dy) \right)^{\frac{1}{c}} \\ &= -\log \|e^{-V(y)}\|_{L_c(\Omega_2)}. \end{aligned}$$

Then, because of the nonnegativity and boundedness of  $V(y)$ ,

$$(4.14) \quad \begin{aligned} \lim_{c \rightarrow \infty} \Lambda_1^-(c) &= \log \|e^{-V(y)}\|_{\infty} \\ &= -\log(e^{\| -V(y) \|_{\infty}}) \\ &= \operatorname{ess\,inf}_{y \in \Omega_2} V(y). \quad \square \end{aligned}$$

Theorem 4.3 ensures that  $\lim_{c \rightarrow \infty} \Lambda_1^+(c)$  is the tightest upper bound for  $\int_{\Omega_1} \mathbb{I}_{\Omega_f}(x, y) \mu(dx)$  for any epistemic variable  $y$  and  $\lim_{c \rightarrow \infty} \Lambda_1^-(c)$  is the tightest lower bound.

**5. Numerical methods.** After introducing and establishing the bounds for the failure probability, we investigate efficient numerical algorithms for computing these bounds. Since the bounds are defined via the exponential integrals in  $\Theta^+$ ,  $\Theta^-$ ,  $\Lambda_1^+$ , and  $\Lambda_1^-$ , it suffices to discuss the computation of these terms. These quantities involve integration of exponential functions in the irregular failure domain, and we will primarily discuss the basic algorithms based on sampling. Other types of methods used in the traditional failure probability computation can potentially be employed, and we will leave those choices to future research.

**5.1. MCS.** MCS is a straightforward way to compute the multidimensional integrals involved in the bounds. For the epistemic case, based on the definitions of  $\Theta^+(c)$  and  $\Theta^-(c)$  in (3.12), we assign a probability measure  $\rho$  to the epistemic variable. By doing so, we give the measure  $\rho$  the role of the nominal, or reference, probability measure. Let  $z^{(i)}$ ,  $i = 1, \dots, M$ , be a set of samples drawn from  $\rho$ , where  $M > 1$  is the number of samples. Then for any  $c > 0$ ,

$$(5.1) \quad \begin{aligned} \Theta^+(c) &\approx \frac{1}{c} \log \left( \frac{1}{M} \sum_{i=1}^M e^{c\mathbb{I}_{\Omega_f}(z^{(i)})} \right), \\ \Theta^-(c) &\approx -\frac{1}{c} \log \left( \frac{1}{M} \sum_{i=1}^M e^{-c\mathbb{I}_{\Omega_f}(z^{(i)})} \right). \end{aligned}$$

Numerical convergence is achieved by increasing the number of samples, i.e.,  $M \rightarrow \infty$ . Note that the same set of samples can be used for any constant  $c$ . This implies that the optimization problems (3.15) and (3.16) do not incur repeated MCS when  $c$  is varied.

For the mixed aleatory and epistemic uncertainty case, we consider  $\Lambda_1^+(c)$  and  $\Lambda_1^-(c)$ , defined in (4.3). Let  $x^{(i)}$ ,  $i = 1, \dots, M_x$ , be samples drawn from the known probability measure  $\mu(x)$  for the aleatory variable  $x$  and  $y^{(j)}$ ,  $j = 1, \dots, M_y$ , be samples drawn from an assigned nominal probability measure  $\rho(y)$  for the epistemic variable  $y$ . The following numerical estimates can be readily employed:

$$(5.2) \quad \begin{aligned} \Lambda_1^+(c) &\approx \frac{1}{c} \log \left( \frac{1}{M_y} \sum_{j=1}^{M_y} e^{\frac{1}{M_x} \sum_{i=1}^{M_x} c\mathbb{I}_{\Omega_f}(x^{(i)}, y^{(j)})} \right), \\ \Lambda_1^-(c) &\approx -\frac{1}{c} \log \left( \frac{1}{M_y} \sum_{j=1}^{M_y} e^{\frac{1}{M_x} \sum_{i=1}^{M_x} -c\mathbb{I}_{\Omega_f}(x^{(i)}, y^{(j)})} \right). \end{aligned}$$

Once these quantities are computed, the bounds from Theorem 3.6 and Theorem 4.1 can be computed via a proper optimization procedure.

**5.2. Surrogate-based hybrid algorithm.** One of the main difficulties of MCS is its simulation cost, as typically a large number of samples are required to obtain accurate estimates of the underlying integrals. Each sample requires a full-scale simulation of a potentially very complex system to decide whether it is “safe” or a “failure.” And one can usually not afford too many samples. In many cases, though, there exists a surrogate model that can approximate the failure function  $g$ , which defines the failure domain  $\Omega_f$  (2.2) with reasonable accuracy. That is, one has an explicitly known function  $\tilde{g} \approx g$ . It is then possible to improve the performance of MCS via the use of  $\tilde{g}$ , because sampling of  $\tilde{g}$  incurs no simulation cost of the underlying system. However, a direct MCS sampling on the surrogate  $\tilde{g}$ , which is the standard approach of the response surface method (RSM), is fundamentally flawed and can lead to erroneous results [10]. To take advantage of the surrogate  $\tilde{g}$ , a hybrid algorithm that combines the standard MCS and RSM can be used. The main idea is to use the samples of  $\tilde{g}$  (which require no simulation effort of the underlying system) “away” from the failure mode  $g = 0$  and then use the samples of the real system “close” to zero. The details of the algorithm, along with its convergence proof and numerical performance, can be found in [10, 9]. Here we only outline its implementation for computing the terms  $\Theta^+$ ,  $\Theta^-$ ,  $\Lambda_1^+$ , and  $\Lambda_1^-$ .

For  $\Theta^+(c)$  and  $\Theta^-(c)$  in (3.12), let  $\rho$  be a nominal probability measure assigned to the epistemic variable. Let  $z^{(i)}$ ,  $i = 1, \dots, M$ , be a set of samples drawn from  $\rho$ , where  $M > 1$  is the number of samples. Then for any  $c > 0$ , we have the following:

Initialization:

- (a) Evaluate  $\tilde{g}(z^{(i)})$ ,  $i = 1, \dots, M$ , and sort the results in ascending order of  $|\tilde{g}(z^{(i)})|$ .
- (b) Set  $P^0 = \frac{1}{M} \sum_{i=1}^M \mathbb{I}_{\{\tilde{g} < 0\}}(z^{(i)})$  as the initial estimate of the failure probability.
- (c) Let  $1 \leq \delta M \ll M$  be the number of samples to be evaluated by the true model in each iterative step and  $\eta \geq 0$  be an error control. Let  $\delta \mathcal{S}^j$  be the set of the  $((j-1)\delta M + 1)$ th sample to the  $(j\delta M)$ th sample in the sorted sample set, where  $j = 1, \dots, \lceil \frac{M}{\delta M} \rceil$ .

At the  $k$ th iterative step ( $k \geq 1$ ):

- (d) (5.3) 
$$P^k = P^{k-1} + \sum_{z \in \delta \mathcal{S}^k} [\mathbb{I}_{\{g < 0\}}(z) - \mathbb{I}_{\{\tilde{g} < 0\}}(z)].$$
- (e) If  $|P^k - P^{k-1}| \leq \eta$ , exit; otherwise, let  $k \leftarrow k+1$ , and repeat the iterative step.

Upon the completion of the iteration, set

$$(5.4) \quad \tilde{\mathbb{I}}(z) = \begin{cases} \mathbb{I}_{\{g < 0\}}(z) & \text{if } z \in \cup_{j=1}^k \delta \mathcal{S}^j; \\ \mathbb{I}_{\{\tilde{g} < 0\}}(z), & \text{otherwise.} \end{cases}$$

Then

$$(5.5) \quad \begin{aligned} \Theta^+(c) &\approx \frac{1}{c} \log \left( \frac{1}{M} \sum_{i=1}^M e^{c\tilde{\mathbb{I}}(z^{(i)})} \right), \\ \Theta^-(c) &\approx -\frac{1}{c} \log \left( \frac{1}{M} \sum_{i=1}^M e^{-c\tilde{\mathbb{I}}(z^{(i)})} \right). \end{aligned}$$

For the mixed aleatory and epistemic case, let  $x^{(i)}$ ,  $i = 1, \dots, M_x$ , be samples drawn from the known probability measure  $\mu(x)$  for the aleatory variable  $x$  and  $y^{(j)}$ ,  $j = 1, \dots, M_y$ , be samples drawn from an assigned nominal probability measure  $\rho(y)$  for the epistemic variable  $y$ . We then repeat the above procedure to determine  $\tilde{\mathbb{I}}$  in (5.4). The terms of  $\Lambda_1^+$  and  $\Lambda_1^-$  can then be readily approximated by

$$(5.6) \quad \begin{aligned} \Lambda_1^+(c) &\approx \frac{1}{c} \log \left( \frac{1}{M_y} \sum_{j=1}^{M_y} e^{\frac{1}{M_x} \sum_{i=1}^{M_x} c\tilde{\mathbb{I}}(x^{(i)}, y^{(j)})} \right), \\ \Lambda_1^-(c) &\approx -\frac{1}{c} \log \left( \frac{1}{M_y} \sum_{j=1}^{M_y} e^{\frac{1}{M_x} \sum_{i=1}^{M_x} -c\tilde{\mathbb{I}}(x^{(i)}, y^{(j)})} \right). \end{aligned}$$

**6. Numerical examples.** In this section we provide a few examples of computing the bounds for failure probability. For benchmarking purposes, the examples here all have analytical expressions for the failure function, as our goal is to examine the behavior of the bounds rather than the performance of the numerical algorithms. All numerical results are obtained by using algorithms based on MCS using a sufficiently large number of samples so that the numerical errors are negligible.

Throughout this section we use  $\mathcal{A}$  to denote the set of probability measures that the epistemic variable can take and  $\rho$  the nominal, or reference, probability measure from which the bounds are computed. The set  $\mathcal{A}$  in all examples is assumed to be a parameterized family of distributions, for example, Gaussian distributions with varying mean and variance. This corresponds to the practical cases where one has a rough idea of the type of distribution of the epistemic variable and is unsure about its precise parameter setting. Note that one can always make  $\mathcal{A}$  a large set to reflect the severe lack of knowledge of the problem. The bounds of the failure probability would inevitably become large. When  $\mathcal{A}$  is sufficiently large, we will obtain the bound of  $0 \leq P_f \leq 1$  without resorting to any estimation techniques, because this is, by definition, the natural bound for  $P_f$ .

**6.1. Example 1: Ordinary differential equation.** Consider a random ODE

$$(6.1) \quad \frac{du}{dt} = -Xu, \quad u(0) = u_0,$$

where  $X$  is a random variable representing the uncertain input and  $u_0$  is the initial condition. The problem admits a trivial analytical  $u(t) = u_0 e^{-Xt}$ , though its availability is immaterial to the computation task we perform here. The failure function is defined as  $g(X) = u_d - u(1)$ , where  $u_d > 0$  is a constant. In all the examples here we fix  $u_0 = 1$  and consider two cases:

- Regular probability. Here we set  $u_d = 4$  and the failure probability  $P_f \sim O(1)$ .
- Small probability. Here we set  $u_d = 70$  and the failure probability  $P_f \sim O(10^{-2})$ .

**6.1.1. Epistemic uncertainty.** In the first set of tests we treat the variable  $X$  as an epistemic variable and restrict its distribution to a set of Gaussian distributions. More specifically, we consider the set of probability measures  $\mathcal{A}$  associated with the following three cases:

- (1a)  $\mathcal{N}(m, 1) : m \in [-2.2, 1.8]$ ,
- (1b)  $\mathcal{N}(-2, \sigma) : \sigma \in [0.9, 1.1]$ ,
- (1c)  $\mathcal{N}(m, \sigma) : m \in [-2.2, -1.8], \sigma \in [0.9, 1.1]$ .

The nominal distribution  $\rho$  is set as  $\mathcal{N}(-2, 1)$ . The bounds are then computed based on Theorem 3.6. The results are summarized in Table 6.1, where  $R^*$  is defined in (3.14). Among these three cases, case (1c) has the “most” uncertainty, as the knowledge of both the mean and the variance is lacking. Naturally case (1c) has the widest bounds compared to the other two cases. In Figure 6.1 we plot the curves of  $\Theta^+(c) + \frac{1}{c}R^*$  and  $\Theta^-(c) - \frac{1}{c}R^*$ , which define the upper bound (3.15) and lower bound (3.16), respectively, for all three cases. The existence of the minima in  $\Theta^+(c) + \frac{1}{c}R^*$  (the upper set of curves) and the maxima in  $\Theta^-(c) - \frac{1}{c}R^*$  (the lower set of curves) is clearly visible, as guaranteed by Proposition 3.7.

Similar cases but with small failure probability are considered, where all the settings in cases (1a), (1b), and (1c) are retained, except that  $u_d$  is set to  $u_d = 70$  so

TABLE 6.1  
Example 1 with epistemic uncertainty for the regular probability case.

Case number	(1a)	(1b)	(1c)
$R^*$	0.02	0.0104	0.0304
Lower bound	0.639	0.665	0.617
Upper bound	0.816	0.793	0.835

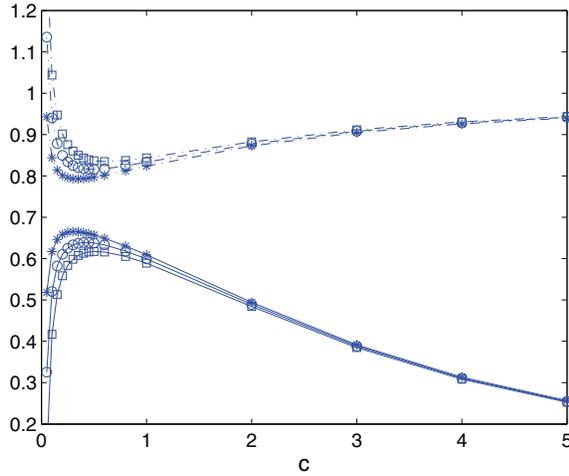


FIG. 6.1. Example 1 with regular probability. Curves of  $\Theta^+(c) + \frac{1}{c}R^*$  (upper set) and  $\Theta^-(c) - \frac{1}{c}R^*$  (lower set) for case (1a) in circles ( $\circ$ ), case (1b) in asterisks ( $*$ ), and case (1c) in squares ( $\square$ ).

TABLE 6.2

Example 1 with epistemic uncertainty for the small-probability case ( $u_d = 70$ ).

Case number	(1a)	(1b)	(1c)
$R^*$	0.02	0.0104	0.0304
Lower bound	0	0.0004	0
Upper bound	0.039	0.031	0.047

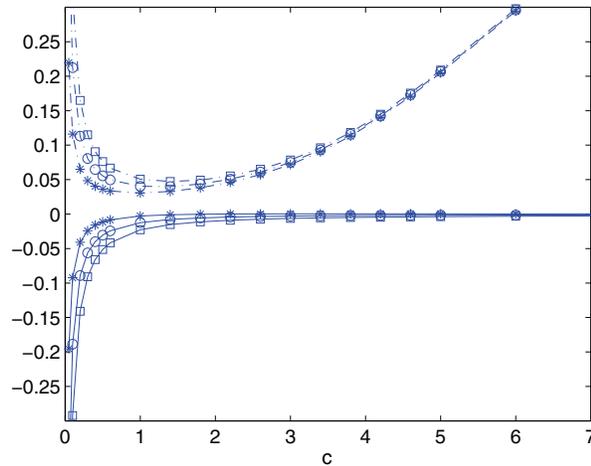


FIG. 6.2. Example 1 with small probability. Curves of  $\Theta^+(c) + \frac{1}{c}R^*$  (upper set) and  $\Theta^-(c) - \frac{1}{c}R^*$  (lower set) for case (1a) in circles ( $\circ$ ), case (1b) in asterisks ( $*$ ), and case (1c) in squares ( $\square$ ).

that the failure probability is of  $O(10^{-2})$ . The results are tabulated in Table 6.2 and also shown in Figure 6.2.

**6.1.2. Mixed aleatory and epistemic uncertainty.** We now modify the settings of the previous section so that the input uncertainty consists of both aleatory and

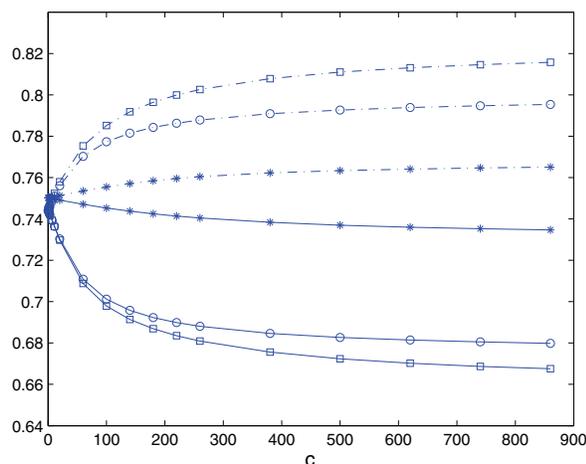


FIG. 6.3. Example 1. Mixed aleatory and epistemic inputs with regular probability ( $u_d = 4$ ). Curves of  $\Lambda_1^+(c)$  (upper set) and  $\Lambda_1^-(c)$  (lower set) for case (2a) in circles (o), case (2b) in asterisks (\*), and case (2c) in squares ( $\square$ ).

TABLE 6.3

Example 1. Mixed aleatory and epistemic inputs with regular probability ( $u_d = 4$ ).

Case number	(2a)	(2b)	(2c)
Lower bound: $\lim_{c \rightarrow \infty} \Lambda_1^-(c)$	0.674	0.729	0.66
Upper bound: $\lim_{c \rightarrow \infty} \Lambda_1^+(c)$	0.8007	0.7687	0.824

epistemic uncertainty. More specifically, we write the input variable as  $X = m + \sigma Z$ , where  $Z$  is an aleatory variable with Gaussian distribution  $\mathcal{N}(0, 1)$ . The following three cases are considered:

- (2a)  $m \in [-2.2, -1.8]$  is epistemic and  $\sigma = 1$  is fixed.
- (2b)  $m = -2$  is fixed and  $\sigma \in [0.9, 1.1]$  is epistemic.
- (2c) Both  $m$  and  $\sigma$  are epistemic with  $m \in [-2.2, -1.8]$ ,  $\sigma \in [0.9, 1.1]$ .

Note that even though these three cases are very similar to those in section 6.1.1, they are different—here the input variable  $X$  might not be Gaussian any more.

For the estimation of the bounds, we employ Theorem 4.3 and compute  $\lim_{c \rightarrow \infty} \Lambda_1^+(c)$  and  $\lim_{c \rightarrow \infty} \Lambda_1^-(c)$ , which are the tightest upper bound and lower bound, respectively, for  $\int \mathbb{I}_{\Omega_f}(x, y) \mu(dx)$ . In all computations we employ uniform distribution as the nominal distribution  $\rho$ . Figure 6.3 shows curves of  $\Lambda_1^+$  (the upper set) and  $\Lambda_1^-$  (the lower set) for all three cases with regular failure probability ( $u_d = 4$  and  $P_f \sim O(1)$ ). The bounds are tabulated in Table 6.3. Again we observe that the bounds of case (2c) are wider because it contains the most uncertainty.

Similar results for the small-probability case, where we set  $u_d = 70$  and  $P_f \sim O(10^{-2})$ , are shown in Figure 6.4 and Table 6.4.

**6.2. Example 2: Bivariate function.** We now consider a relatively more practical example. The failure function is defined as

$$(6.2) \quad g = u(X_1, X_2, \eta)/2 - 1 - g_d,$$

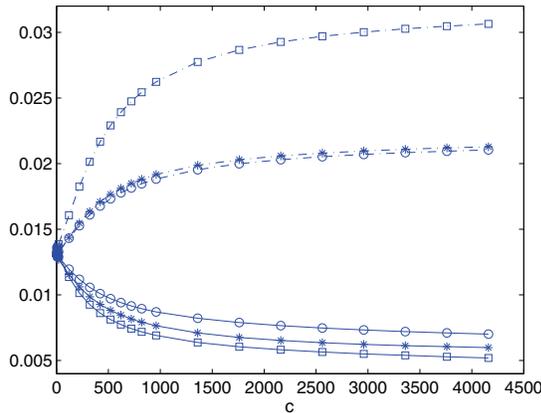


FIG. 6.4. Example 1. Mixed aleatory and epistemic inputs with small probability ( $u_d = 70$ ). Curves of  $\Lambda_1^+(c)$  (upper set) and  $\Lambda_1^-(c)$  (lower set) for case (2a) in circles ( $\circ$ ), case (2b) in asterisks ( $*$ ), and case (2c) in squares ( $\square$ ).

TABLE 6.4

Example 1. Mixed aleatory and epistemic inputs with regular probability ( $u_d = 70$ ).

Case number	(2a)	(2b)	(2c)
Lower bound: $\lim_{c \rightarrow \infty} \Lambda_1^-(c)$	0.006	0.0053	0.0037
Upper bound: $\lim_{c \rightarrow \infty} \Lambda_1^+(c)$	0.022	0.023	0.0323

where  $X_1, X_2$  are two random variables and  $u$  is defined by the following nonlinear system of equations:

$$(6.3) \quad \begin{aligned} u(X_1, X_2, \eta) &= X_1^2 + \eta - 0.2v(X_1, X_2, \eta), \\ v(X_1, X_2, \eta) &= \sqrt{u(X_1, X_2, \eta)} + X_1 + X_2. \end{aligned}$$

We set  $\eta = 1.5$  and assume  $X_1$  is an aleatory random variable of  $\mathcal{N}(0.9, 0.5)$  and  $X_2$  is an epistemic variable taking values on the interval  $[0, 1]$ . We employ two values for  $g_d$ :  $g_d = 0$  results in the regular probability case  $P_f \sim O(1)$ , and  $g_d = -0.45$  results in the small-probability case  $P_f \sim O(10^{-2})$ . We also construct high-order polynomial expansions to the functions  $u$  and  $v$ , using the generalized polynomial chaos strategy (see [14] for details), and use the polynomial approximations as surrogate models to facilitate the computation of the bounds (see section 5.2).

We first compute the quantities  $\Lambda_1^+(c)$  and  $\Lambda_1^-(c)$ , as defined in (4.3), by setting the nominal probability measure  $\rho$  to be uniform in  $[0, 1]$ . The curves of  $\Lambda_1^+$  and  $\Lambda_1^-$  are shown in Figure 6.5. By taking the limit of  $c \rightarrow \infty$ , we obtain the tightest bounds for  $\int \mathbb{I}_{\Omega_f}(x_1, x_2)\mu(dx_1)$  for any  $X_2 \in [0, 1]$ . For the regular probability case,  $0.580 \leq \int \mathbb{I}_{\Omega_f}(x_1, x_2)\mu(dx_1) \leq 0.655$ , and for the small-probability case,  $0 \leq \int \mathbb{I}_{\Omega_f}(x_1, x_2)\mu(dx_1) \leq 0.068$ .

Next we assume that the “true” distribution  $\gamma$  of the epistemic variable  $X_2$  belongs to the set of probability measures  $\mathcal{A}$  associated with the beta distribution  $B(\alpha, \beta)$  with  $\alpha \in [1, 1.5]$  and  $\beta \in [1, 1.5]$ . We employ Theorem 4.1 to compute the bounds and plot the curves of  $\Lambda_1^+(c) + \frac{1}{c}R^*$  and  $\Lambda_1^-(c) - \frac{1}{c}R^*$  in Figure 6.6, where  $R^* = \sup_{\gamma \in \mathcal{A}} R(\gamma(dx_2) \parallel \rho(dx_2)) \approx 0.0721$ . The bounds are the minima and maxima of these curves—for the regular probability case,  $0.611 \leq P_f \leq 0.627$ , and for the small-probability case,  $0.0005 \leq P_f \leq 0.012$ .

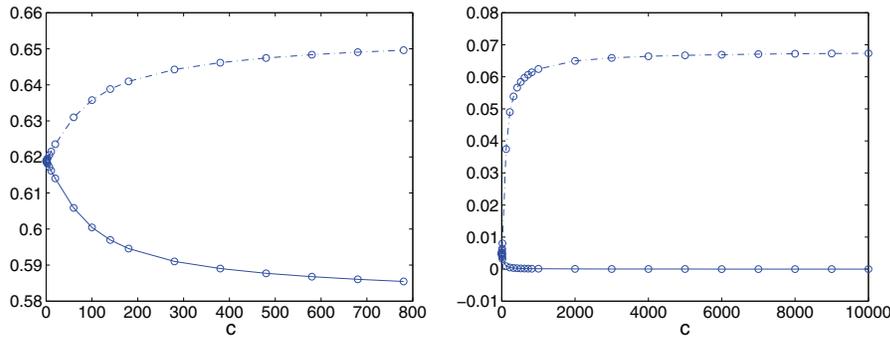


FIG. 6.5. Example 2. Curves of  $\Lambda_1^+(c)$  (dashed line) and  $\Lambda_1^-(c)$  (solid line). Left: regular probability case with  $g_d = 0$ ; right: small-probability case with  $g_d = -0.45$ .

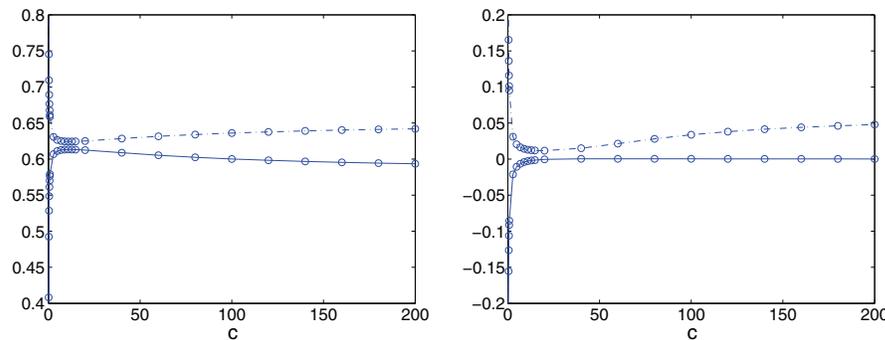


FIG. 6.6. Example 2. Curves of  $\Lambda_1^+(c) + \frac{1}{c}R^*$  (dashed line) and  $\Lambda_1^-(c) - \frac{1}{c}R^*$  (solid line). Left: regular probability case with  $g_d = 0$ ; right: small-probability case with  $g_d = -0.45$ .

**6.3. Example 3: Multivariate example.** We now consider a multivariate example, which was used in [10] as well. The failure function is defined as

$$(6.4) \quad g(X) = X_1 + 2X_2 + 2X_3 + X_4 - 5X_5 - 5X_6 + 0.001 \sum_{i=1}^6 \sin(100X_i) - g_d,$$

where  $X_i \sim LN(m_i, \sigma_i)$  for  $i = 1, \dots, 6$  are log-normal random variables and  $g_d$  is a real parameter.

We assume that  $Z_i = \log(X_i)$ ,  $i = 1, \dots, 5$  are aleatory variables;  $m_1 = 120, \sigma_1 = 12$ ;  $m_2 = 120, \sigma_2 = 12$ ;  $m_3 = 120, \sigma_3 = 12$ ;  $m_4 = 120, \sigma_4 = 12$ ;  $m_5 = 50, \sigma_5 = 5$ ; and  $Z_6$  is an epistemic variable. Let  $Z_6 = \log(X_6) \sim \mathcal{N}(\hat{m}_6, \hat{\sigma}_6)$ . We choose a Gaussian distribution  $\mathcal{N}(m^*, \sigma^*)$  as the nominal probability measure  $\rho$  of  $Z_6$  such that  $X_6$  is  $LN(40, 6)$ . We then construct the following three cases:

TABLE 6.5  
Example 3 for regular probability case with  $g_d = 250$ .

Case number	(3a)	(3b)	(3c)
$R^*$	0.0022	0.0189	0.0211
Bounds by (3.17)	[0.321, 0.385]	[0.262, 0.488]	[0.257, 0.453]
Bounds by (4.9)	[0.339, 0.366]	[0.342, 0.363]	[0.326, 0.373]

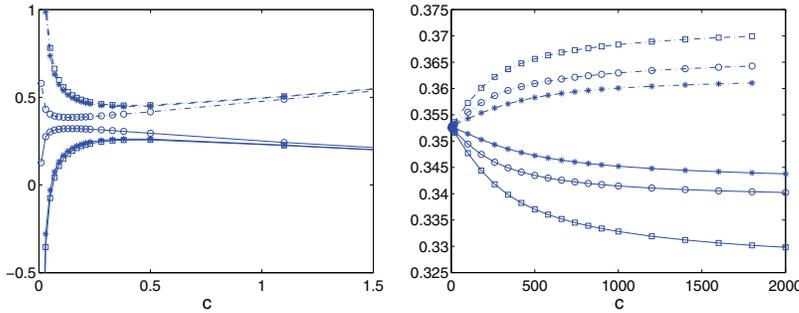


FIG. 6.7. Example 3. Regular probability with  $g_d = 250$ , for case (3a) in circles ( $\circ$ ), case (3b) in asterisks ( $*$ ), and case (3c) in squares ( $\square$ ). Left: curves of  $\Theta^+(c) + \frac{1}{c}R^*$  (upper set) and  $\Theta^-(c) - \frac{1}{c}R^*$  (lower set); right: curves of  $\Lambda_1^+(c)$  (upper set) and  $\Lambda_1^-(c)$  (lower set).

TABLE 6.6  
Example 3 for small-probability case with  $g_d = 150$ .

Case number	(3a)	(3b)	(3c)
$R^*$	0.0022	0.0189	0.0211
Bounds by (3.17)	[0.0076, 0.0238]	[0, 0.044]	[0, 0.046]
Bounds by (4.9)	[0.0127, 0.0163]	[0.0093, 0.0213]	[0.0087, 0.0237]

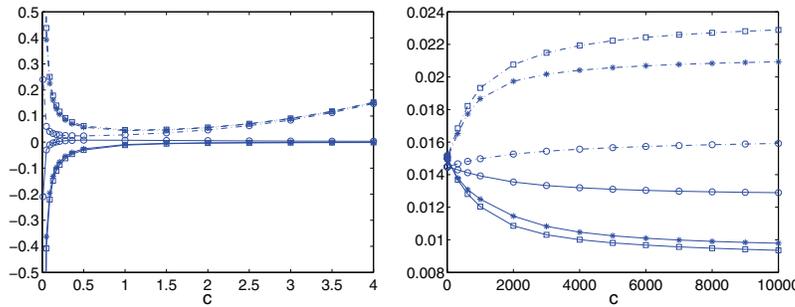


FIG. 6.8. Example 3. Small probability with  $g_d = 150$ , for case (3a) in circles ( $\circ$ ), case (3b) in asterisks ( $*$ ), and case (3c) in squares ( $\square$ ). Left: curves of  $\Theta^+(c) + \frac{1}{c}R^*$  (upper set) and  $\Theta^-(c) - \frac{1}{c}R^*$  (lower set); right: curves of  $\Lambda_1^+(c)$  (upper set) and  $\Lambda_1^-(c)$  (lower set).

- (3a)  $\hat{m}_6 \in [m^* - 0.01, m^* + 0.01]$  and  $\hat{\sigma}_6 = \sigma^*$ .
- (3b)  $\hat{m}_6 = m^*$ , and  $\hat{\sigma}_6 \in [\sigma^* - 0.02, \sigma^* + 0.02]$ .
- (3c)  $(\hat{m}_6, \hat{\sigma}_6) \in [m^* - 0.01, m^* + 0.01] \times [\sigma^* - 0.02, \sigma^* + 0.02]$ .

To compute the bounds, we construct a multidimensional Hermite polynomial approximation to  $X_1 + 2X_2 + 2X_3 + X_4 - 5X_5 - 5X_6$  and employ it as a surrogate. (Note that the surrogate model neglects the summation term.) The surrogate-based hybrid algorithm is then used to compute the bounds, as described in section 5.2.

Once again, we compute two types of bounds. The first set of bounds are from Theorem 3.6, obtained by finding the minimum of  $\Theta^+(c) + \frac{1}{c}R^*$  and the maximum of  $\Theta^-(c) - \frac{1}{c}R^*$ . The second set of bounds are obtained by considering the mixed aleatory and epistemic uncertainty and using Theorem 4.3 to find the limits of  $\Lambda_1^+(c)$  and  $\Lambda_1^-(c)$ . The results are shown in Table 6.5 and Figure 6.7 for the regular probability case with  $g_d = 250$ , and in Table 6.6 and Figure 6.8 for the small-probability case with  $g_d = 150$ .

**7. Summary.** In this paper we develop rigorous methods to estimate both the upper and lower bounds for failure probability computation in the presence of epistemic uncertainty. The results will be useful in practical situations where one does not have sufficient information about the probability distributions of the uncertain inputs. The proposed methods will enable practitioners to reliably estimate the “best-case scenario” and the “worst-case scenario” for failure probability computations.

## REFERENCES

- [1] X. CHEN, E.-J. PARK, AND D. XIU, *A flexible numerical approach for quantification of epistemic uncertainty*, J. Comput. Phys., submitted.
- [2] K. CHOWDHARY AND P. DUPUIS, *Distinguishing and integrating aleatoric and epistemic variation in uncertainty quantification*, ECIAM M2M, submitted (2011).
- [3] D. DUBOIS AND H. PRADE, *Possibility Theory: An Approach to Computerized Processing of Uncertainty*, Plenum, New York, 1998.
- [4] P. DUPUIS AND R. S. ELLIS, *A Weak Convergence Approach to the Theory of Large Deviations*, John Wiley & Sons, New York, 1997.
- [5] M. ELDRED, L. SWILDER, AND G. TANG, *Mixed aleatory-epistemic uncertainty quantification with stochastic expansions and optimization-based interval estimation*, Reliab. Eng. Sys. Safety, 96 (2011), pp. 1092–1113.
- [6] J. C. HELTON, J. D. JOHNSON, W. L. OBERKAMPF, AND C. J. SALLABERRY, *Representation of Analysis Results Involving Aleatory and Epistemic Uncertainty*, Technical Report 4379, Sandia National Laboratories, 2008.
- [7] J. C. HELTON, J. D. JOHNSON, W. L. OBERKAMPF, AND C. B. STORLIE, *A Sampling-Based Computational Strategy for the Representation of Epistemic Uncertainty in Model Predictions with Evidence Theory*, Technical Report 5557, Sandia National Laboratories, 2006.
- [8] J. JAKEMAN, M. ELDRED, AND D. XIU, *Numerical approach for quantification of epistemic uncertainty*, J. Comput. Phys., 229 (2010), pp. 4648–4663.
- [9] J. LI, J. LI, AND D. XIU, *An efficient surrogate-based method for computing rare failure probability*, J. Comput. Phys., 230 (2011), pp. 8683–8697.
- [10] J. LI AND D. XIU, *Evaluation of failure probability via surrogate models*, J. Comput. Phys., 229 (2010), pp. 8966–8980.
- [11] L. J. LUCAS, H. OWHADI, AND M. ORTIZ, *Rigorous verification, validation, uncertainty quantification and certification through concentration-of-measure inequalities*, Comput. Methods Appl. Mech. Engrg., 197 (2008), pp. 4591–4609.
- [12] L. SWILER, T. PAEZ, R. MAYES, AND M. ELDRED, *Epistemic uncertainty in the calculation of margins*, in Proceedings of the AIAA Structures, Structural Dynamics, and Materials Conference, Palm Springs, CA, May 2009.
- [13] L. P. SWILER, T. L. PAEZ, AND R. Q. L. MAYES, *Epistemic uncertainty quantification tutorial*, in Proceedings of the IMAC XXVII Conference and Exposition on Structural Dynamics, Orlando, FL, February 2009.
- [14] D. XIU, *Numerical Methods for Stochastic Computations*, Princeton University Press, Princeton, NJ, 2010.