Machine Learning-Based Hybrid Random-Fuzzy Modeling Framework for Antenna Design

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***Abstract*—A machine learning-based framework is proposed to evaluate the effect of design parameters, affected by both aleatory and epistemic uncertainty, on the performance of antennas. In particular, possibility theory is leveraged to define aleatory and epistemic uncertainty in a common framework. Then, a method combining Bayesian optimization and Polynomial Chaos expansion is applied to accurately and efficiently propagate both uncertainties throughout the system under study. A suitable application example validates the proposed method.**

***Index Terms*—Bayesian optimization, epistemic uncertainty, Gaussian process, random-fuzzy problems.**

I. Introduction

Uncertainty quantification (UQ) for antenna design is typically performed through statistical methods. Among these, the traditional approach resorts to Monte Carlo (MC) analysis, which requires a high number of simulations of the antenna under study. Another method is the Polynomial Chaos (PC) expansion [1]–[6], which models the variations in antenna performance in terms of stochastic surrogates.

All these approaches are solidly based on probability theory. Namely, the design parameters subject to uncertainty are considered random variables, which are characterized by probability distributions [7]–[9]. These distributions can be chosen *a priori* over a given interval and/or around a nominal value. However, assuming that all the design parameters are affected by aleatory uncertainty, as described by probabilistic frameworks, is not always a reliable approach. As a matter of fact, when the uncertainty stems from lack of knowledge about the value and/or variability of a parameter over a certain interval, possibility theory [10] offers a more adequate framework for representing such an epistemic uncertainty. An epistemic UQ approach for textile antenna designs is presented in [11]. However, in more complex scenarios, design parameters affected by both aleatory and epistemic uncertainties are present. In this case, a hybrid approach is necessary to tackle the UQ problem.

In this contribution, we present a machine learning-based framework for the solution of hybrid probabilistic-possibilistic UQ problems: design parameters that suffer from aleatory uncertainty effects (random variables) are assigned probability distribution functions (PDFs), whereas design parameters affected by epistemic uncertainty (fuzzy variables) are assigned possibility distributions (PDs). Bayesian Optimization (BO) is exploited to propagate epistemic uncertainty, and PC expansion to deal with aleatory uncertainty. Efficiency and accuracy of the presented hybrid algorithm are validated by a suitable application example.

The manuscript is organized as follows. First, in Section II, the relevant features of possibility theory are presented, and the main features of standard hybrid probabilistic-possibilistic algorithms are described. Section III briefly introduces BO, and the procedure to apply BO to the possibilistic part of the algorithm. Also, the hybridization of BO with the PC method to speed up the UQ problem is discussed. An application example is presented in Section IV. Conclusions are drawn in Section V.

II. FORMULATION OF THE HYBRID POSSIBILISTIC-PROBABILISTIC PROBLEM

The relevant features of possibility theory as a general framework to represent both aleatory and epistemic uncertainty are introduced in Section II-A, whereas the current standard approach to joint UQ of possibilistic and probabilistic information is briefly explained in Section II-B.

A. *Possibility Theory and Epistemic Uncertainty*

While probability theory describes random variables (aleatory uncertainty) through probability distribution functions, it falls short in representing variables affected by epistemic uncertainty. To overcome this limitation, the more general framework of possibility theory and fuzzy variables was introduced [10].

In this framework, a real valued parameter x is characterized by a possibility distribution (PD) $\pi(x)$ such that:

$$\pi : \mathbb{R} \rightarrow [0,1], \exists\, x \in \mathbb{R} : \pi(x) = 1. \tag{1}$$

While a PDF represents the frequency of occurrence of an event over a certain interval, a PD represents the likelihood that a value x may assume. Hence, the set $[0,1]$ corresponds to different level of confidence assigned to each value of x. For instance, 0 corresponds to an impossible value, and 1 corresponds to a perfectly possible value.

Many PDs can be defined, among which the most commonly used are the rectangular and the triangular ones. Rectangular

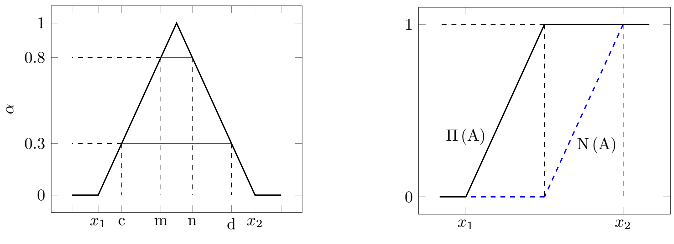

Figure 1: (a) A triangular PD, $\pi(x)$, and (b) the corresponding possibility Π (solid) and necessity N (dashed) measures.

PDs typically represent the so-called total ignorance, that is the case in which no information on the variability of a parameter is available [12]. In this case, all the values in the interval $[x_1, x_2]$ are equally possible, and the confidence level assigned to all values in this interval is equal to 1. Triangular PDs, on the other hand, are suited when a higher degree of confidence can be assigned to one value in the interval, and the confidence level for all the other values decreases gradually (see Fig. 1(a)).

According to the theory of fuzzy sets, an epistemic (or fuzzy) variable x can also be fully characterized by its α-cuts. The α-cuts of a fuzzy variable are intervals obtained by cutting its PD at different α levels (with α ranging from 1 to 0). In Fig. 1(a), two α-cuts (red lines) of a triangular PD are shown. The α-cut at level 0.3 is the interval $[c, d]$, whereas the α-cut at level 0.8 is the interval $[m, n]$.

Eventually, starting from the PD $\pi(x)$, possibility and necessity measures $\Pi(\mathrm{A})$ and $\mathrm{N}(\mathrm{A})$ of a subset $\mathrm{A} \in \mathbb{R}$ are defined as:

$$\Pi(A) = \sup_{x \in A} \pi(x)\,; \quad \mathrm{N}(A) = 1 - \sup_{x \notin A} \pi(x)\,. \tag{2}$$

For the subset $\mathrm{A} = (-\infty, x]$, the relationship between the PD $\pi(x)$ of a continuous uncertain variable x and its corresponding possibility Π and necessity N measures is illustrated in Fig. 1.

Given the subset A, it was proven that $\Pi(\mathrm{A})$ and $\mathrm{N}(\mathrm{A})$ represent the upper and lower bounds of all possible cumulative distribution functions (CDFs) $P(\mathrm{A})$, such that the relation $\mathrm{N(A)} \leq P(\mathrm{A}) \leq \Pi(\mathrm{A})$ holds [13], [14].

B. Uncertainty Propagation (UP) in Hybrid Possibilistic-Probabilistic Problems

Hybrid probabilistic-possibilistic problems are characterized by the coexistence of aleatory and epistemic uncertainty. Taking their different meaning and behaviour into account, aleatory uncertainty is characterized by PDFs p, whereas epistemic uncertainty is modelled by PDs π. Several approaches have been proposed in literature to UP in such hybrid problems, most of them resorting to "brute force" approaches and requiring a very dense sampling of the input space.

Consider a function f depending on a total number of M variables: T of theme are random variables $r_1, r_2, ..., r_T$, and $T - M$ are epistemic variables $f_{T+1}, f_{T+2}, ..., f_M$, as $f(r_1, ..., r_T, f_{T+1},, ..., f_M)$. Propagation and quantification of the uncertainty of the function f encompass the following steps.

1) A number of realizations of the T random variables are generated.
2) For a predetermined number of α-cuts ranging from α=1 to α=0, f is evaluated for each α-cut on a dense grid in the space of epistemic variables.
3) The f_{min} and the f_{max} of the function f at different α levels are as such determined in a brute-force way, and denoted Inf_α and Sup_α. These minimum and maximum values construct the PD π associated with a specific random-variable realization.
4) This procedure is repeated for all random-variable realizations and the resulting distributions are obtained via aggregation.

For the above-described algorithm, it is straightforward that solution based on "brute force" methods may become computationally inefficient even for a small number of random-fuzzy variables. This issue is especially relevant for electromagnetic (EM) problems, where the objective function f is often evaluated through computationally-expensive full-wave simulations. To overcome these limitations, in the following Section a machine learning-based approach will be presented, which combines BO and PC expansion methods.

III. PROPOSED METHODOLOGY

In this Section, after a brief introduction of BO basic concepts [15], the procedure of employing BO to propagate the epistemic uncertainty in the previously-introduced hybrid algorithm is explained. Eventually, Section III-C describes the hybridization of BO with PC to effectively manage the part of the algorithm pertinent to random variables.

A. Overview of Bayesian Optimization

BO is aimed at solving global optimization problems of the form

$$\min_{\mathbf{x} \in \mathrm{X} \subset \mathbb{R}^D} f(\mathbf{x}), \tag{3}$$

where D is the number of design parameters $\mathbf{x}$. The main idea in BO is to perform the minimization (or maximization) on surrogate models that mimic the actual optimization problem but, compared to the latter, are cheaper to evaluate. The flowchart of the BO algorithm is shown in Fig. 2. First, the objective function $f(\mathbf{x})$ is evaluated over an initial set of design parameters $[\mathbf{x}_\mathrm{k}]_{\mathrm{k}=1}^{\mathrm{K}} \in \mathrm{X}$ (chosen, e.g., according to a Latin hypercube). Then, a stochastic surrogate model of $f(\mathbf{x})$ is built based on these initial samples. Since the surrogate model is cheap to evaluate, it is used by the optimizer to determine the location of the candidate optimum. If the distance between the selected point and the previously evaluated one is below a certain threshold, convergence is reached and the optimization is finished. Otherwise, this optimum is evaluated through a new (expensive) simulation. The surrogate model is updated until the computational budged is spent. Hence, each additional simulation refines the surrogate model, increasing

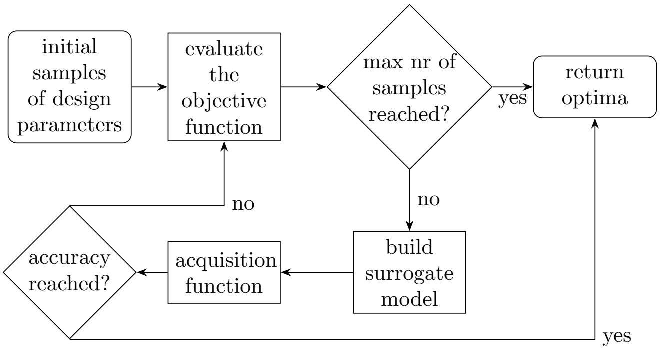

Figure 2: Flowchart of the BO algorithm.

the probability of finding the solution of the optimization problem (3).

For the surrogate model, Gaussian processes (GP) [16] are adopted in this work, owing to their analytic inference, accuracy and modeling power. In particular, the Matérn (5/2) kernel was chosen as GP kernel, due to its capability to model a wide class of functions (including non-differentiable ones). The surrogate model in BO, contrary to other surrogate-based optimization techniques, is *stochastic*. Therefore, the model uncertainty is used to determine a sampling strategy called 'acquisition function' in the BO framework. Among the available acquisition functions, in this work the Expected Improvement (EI) [17] is adopted as sampling method. EI is defined as

$$\mathrm{E}\left[\mathrm{I}\left(\mathbf{x}\right)\right]=\mathrm{E}\left[\max\{0, f_{\min}-y\}\right] \tag{4}$$

where E is the expectation operator, $I\left(\mathbf{x}\right)$ is a suitable measure of improvement defined at the point $\mathbf{x}$, $f_{\min}$ is the current evaluated minimum of the objective function and y is the prediction of the GP surrogate model at point $\mathbf{x}$. Since y is a Gaussian random variable, the expectation in (4) can be calculated analytically. Moreover, the hyper-parameters σ^2 and ρ are optimized using maximum likelihood estimation via the GPyOpt package [18].

B. BO for the Possibilistic Part of the Hybrid Problem

As explained in Section II-B, brute force methods are commonly used for UP in hybrid problems. For example, grid search (GS) method can be used to sample the space of epistemic variables, whereas the Monte Carlo technique can be employed to sample the space of random variables [19]. Another approach consists in using Monte Carlo for both random and epistemic variables. In this work, we have replaced the brute force methods by BO for the possibilistic part of the hybrid algorithm.

BO is particularly suitable for the solution of possibilistic optimization problems where both $\inf_\alpha$ and $\sup_\alpha$ of all α-cuts need to be calculated for each realization of the RVs. A possibility distribution is then constructed with these extreme values. To this purpose, the acquisition function (4) is modified as:

$$\mathrm{EI}_{\mathrm{mm}}\left(\mathbf{x}\right)=\max\{\mathrm{E}\left[\max\{0, f_{\min}-y\}\right], \mathrm{E}\left[\max\{0, y-f_{\max}\}\right]\} \tag{5}$$

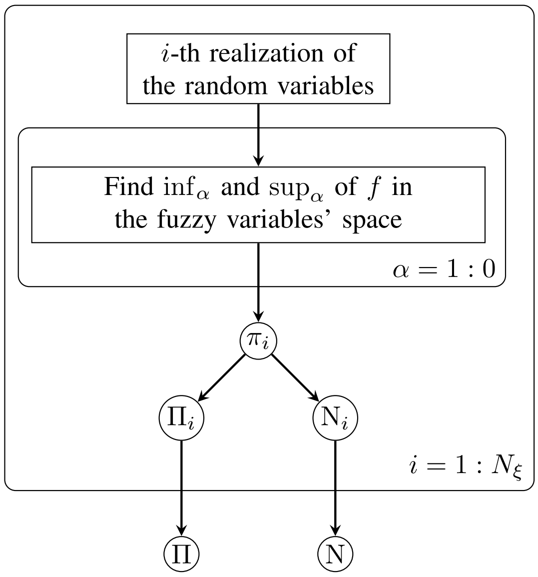

Figure 3: Flowchart of the proposed hybrid algorithm.

This modification allows us to calculate the candidate points in the space of the design parameters with a higher potential of finding a minimum and a maximum at the same time. Indeed, as illustrated by the example in Section IV, the proposed method is capable of finding both optima with a minimal number of evaluations of the objective function $f\left(\mathbf{x}\right)$.

Because α-cuts are always nested, regardless of the specific PD under consideration, BO is performed as follows. First, for a small number of initial samples, BO is applied at the top alpha level (α=1). Next, the optimization for all other α levels is performed progressively by making use of the samples already evaluated at the "upper" α levels and by evaluating only a few additional samples at each subsequent α level. Optimization of the objective function at all α levels is performed until the bottom α level ($\alpha = 0$) is reached. During this process, if a better optimum is found in the current α level, the optimum for previous levels can be updated accordingly, whenever applicable.

C. Joint UP with BO and PC

BO significantly accelerates the solution of the epistemic sub-problems which already reduces the CPU-time of the hybrid algorithm. However, the brute force methods employed for the probabilistic part of the hybrid algorithm, still slow down the hybrid method. To make the hybrid approach more efficient, we replace the brute force MC method by PC expansions [1]. Because of their accuracy and efficiency, PC expansions are widely used for stochastic modeling. A suitable model is built for both the minimum and the maximum of the objective function with respect to the RVs and the α-cuts, as follows:

$$F_{\min}(\alpha, \boldsymbol{\xi}) = \sum_{k=0}^{K} \beta_{\min,k}(\alpha)\,\phi_k(\boldsymbol{\xi}),$$
$$F_{\max}(\alpha, \boldsymbol{\xi}) = \sum_{k=0}^{K} \beta_{\max,k}(\alpha)\,\phi_k(\boldsymbol{\xi}), \quad (6)$$

where $\phi_k(\boldsymbol{\xi})$ are suitable orthogonal polynomials, dependent on the random variables $\boldsymbol{\xi}$, $(k = 0, \ldots, K)$. $\beta_{\min,k}(\alpha)$ and $\beta_{\max,k}(\alpha)$ are the corresponding PC coefficients, depending on the α-cut [1].

Note that the PC basis functions in (6) depend only on the PDFs of the RVs $\boldsymbol{\xi}$, and can be calculated in advance for different distributions [6]. Therefore, only the $\beta_{\min,k}$ and $\beta_{\min,k}$ must be predicted as follows: first, a number of collocations points $[\boldsymbol{\xi}_i]_{i=1}^{N_{PC}}$ are determined in the random variables' space, according to the method reported in [5]. Second, BO is performed at each of the collocation points in order to find the minima and maxima of the cost function with respect to different α-cuts. Then, the desired PC coefficients are calculated by solving a suitable linear system [5]. $F_{\min}$ and $F_{\max}$ at each of the α-cuts and for a specific instance of the random variables $\boldsymbol{\xi}_i$ define the possibility distribution π_i of the objective function f. Thereto, a family of possibility distributions is constructed by computing $F_{\min}$ and $F_{\max}$ (6) for a number of N_ξ MC samples of the RVs. Finally, based on the resulting distributions, the Π and N measures are computed using the aggregation method reported in [20]. The idea here is to evaluate the spread of the output for every α-cut by computing the corresponding CDF based on all the Π and N and by choosing a quantile q. The final result will be an interval for each α-cut that describes the behaviour of the $(q \cdot 100)$ % of the curves coming from simulation. The flowchart of the hybrid algorithm is shown in Fig. 3.

IV. APPLICATION EXAMPLE

In this Section, the hybrid probabilistic-possibilistic method is applied to the dual-polarized textile patch antenna presented in [21] (see Fig. 4). The antenna operates in the $[2.4, 2.4835]$ GHz ISM band. The substrate permittivity ϵ_r and height h are regarded as epistemic variables defined in the intervals $[1.43, 1.63]$ and $[3.44, 4.44]$ mm, respectively. A uniform PD is assigned to the height, whereas a triangular PD is chosen for the relative permittivity. Moreover, the patch width W and length L are regarded as random parameters with $W \sim \mathcal{N}(45.385, 0.1268)$ and $L \sim \mathcal{N}(44.515, 0.1627)$, respectively [22]. Here, $\mathcal{N}(\mu, \sigma)$ is the Gaussian distribution with mean μ and standard deviation σ. The purpose is to estimate the uncertainty of the antenna's scattering parameters at a frequency of 2.4557 GHz. To calculate these scattering parameters, the Momentum electromagnetic field simulator of Advanced Design System (ADS) [23] is adopted.

To compute the PC model coefficients in (6), BO is performed for $K = 10$ samples of the random variables (W, L). In particular, 36 α-cuts ranging from possibility level 1 to 0 are considered for each collocation point. BO starts with 11 (h, ϵ_r) samples at $\alpha = 1$, while 2 additional samples are selected for each following α level, for a total maximum computational budget of 81 (h, ϵ_r) samples. After estimating the PC model coefficients at each α level via BO, a PC model is computed with polynomials up to the third order, for both the minimum and maximum of the scattering parameters $|S_{11}|$ and $|S_{21}|$. Then, PC models are evaluated for 1000 MC samples drawn from the RVs' distributions. Finally, the hybrid outputs are aggregated and the resulting possibility and necessity functions are presented in Figs. 5 and 6 for $|S_{11}|$ and $|S_{21}|$, respectively. The elapsed time is 4.3 hours for this method, using a personal

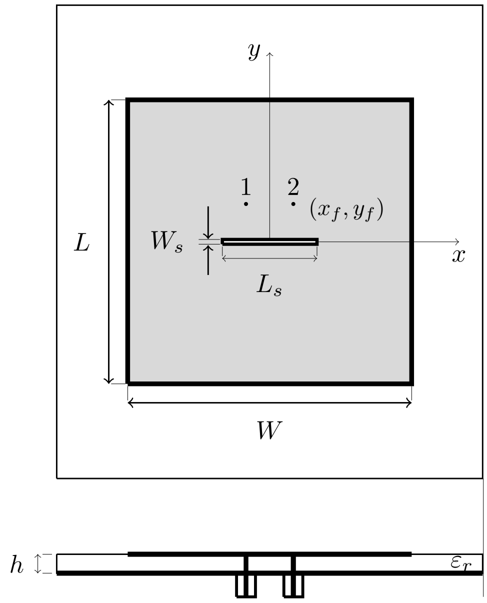

Figure 4: Geometry of the antenna under study. Nominal values: substrate height $h = 3.94$ mm, substrate relative permittivity $\epsilon_r = 1.53$, patch width $W = 45.32$ mm, patch length $L = 44.46$ mm.

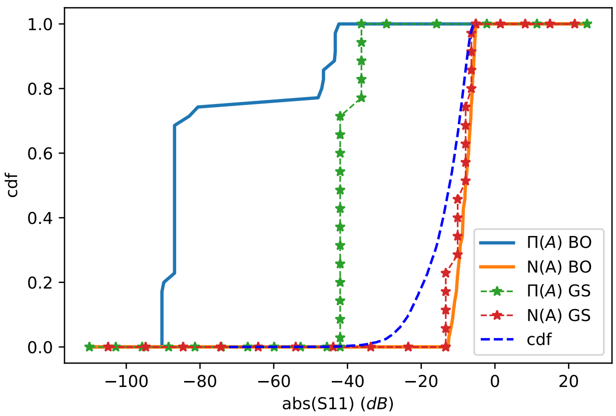

Figure 5: Possibility and Necessity functions of the magnitude of S_{11} (dB) at 2.4557 GHz estimated with PC (random variables) and BO (epistemic variables) are shown with solid lines. The same functions computed with the approach presented in [19] are displayed with stars. Additionally, the blue dashed line indicates the obtained CDF.

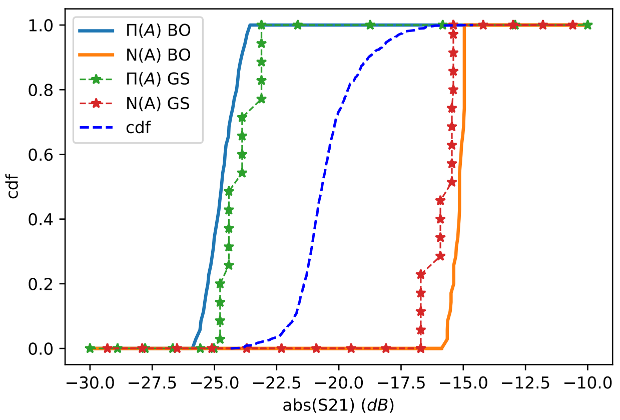

Figure 6: Possibility and Necessity functions of the magnitude of S_{21} (dB) at 2.4557 GHz estimated with PC (random variables) and BO (epistemic variables) are shown with solid lines. The same functions computed with the approach presented in [19] are displayed with stars. Additionally, the blue dashed line indicates the CDF obtained.

computer with 8 GB and 8 cores Intel(R) Core(TM) i7-2600 CPU @ 3.40GHz.

For comparison, the same example was also solved following the procedure adopted in [19]. The corresponding Π and N measures are displayed in Figs. 5 and 6. In particular, the objective function was evaluated for a uniform grid of 9 $\times$ 9 (h, ϵ_r) samples and 1000 (W, L) MC samples, and the elapsed time is 233.4 hours. Results show that for the same number of samples, the proposed BO-PC approach provides a more efficient and accurate solution to the hybrid random-fuzzy problem.

Additionally, a CDF calculated with 10000 (h, ϵ_r, L, W) samples by treating all variables as probabilistic is shown as a blue dashed line in Figs. 5 and 6. In this example, the parameters h and ϵ_r were assigned uniform distributions in the intervals $[3.44, 4.44]$ mm and $[1.43, 1.63]$, respectively. As pointed out in Section II-A, the CDF is always in the domain defined by the possibility and necessity functions.

V. CONCLUSION

A hybrid machine learning-based framework to propagate both aleatory and epistemic uncertainties in antenna design is presented in this contribution. The method leverages the framework of the theory of evidence, to address both probabilistic and possibilistic definitions of uncertainty. Moreover, the proposed algorithm speeds up standard hybrid algorithms by adopting a BO framework for the possibilistic part of the algorithm. To include random variability, PC expansions are successfully hybridized with BO. The presented hybrid UQ method assures higher computational efficiency and better prediction accuracy than standard solution approaches (mostly resorting to repeated simulations and grid-search algorithms), as it was shown by means of a suitable application example.

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