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***Abstract*—The PC-Kriging metamodeling method is proposed for yield estimation of multi-band patch antennas. PC-Kriging is a combination of polynomial chaos expansion (PCE) and Kriging metamodeling, where PCE is used as a trend function for the Kriging interpolation metamodel. The method is demonstrated on the Ishigami analytical function and a dual-band patch antenna. The PC-Kriging is shown to reach the prescribed accuracy limit with significantly fewer training points than both PCE and Kriging. This translates into considerable computational savings of yield estimation over alternative metamodel-based procedures and direct EM-driven Monte Carlo simulation. The saving are obtained without compromising evaluation reliability.**

Keywords—Dual-band patch antenna, yield estimation, polynomial chaos expansion, Kriging, PC-Kriging.

I. Introduction

Manufacturing tolerances, especially those pertinent to geometry parameters may seriously affect performance of the antenna systems. Accounting for these requires uncertainty quantification. One of the important metrics is the yield [1], i.e., the expected percentage of designs that satisfy the prescribed performance requirements [2]. Because reliable antenna evaluation can only be achieved through expensive full-wave electromagnetic (EM) analysis [3], conventional statistical analysis (e.g., Monte Carlo simulations [4]) necessarily involving massive EM simulations is computational prohibitive.

The cost-related difficulties can be alleviated by metamodel-assisted techniques such as response surface approximation (RSA) [5], Kriging metamodel [6], Gradient Enhanced Kriging [7], and polynomial chaos expansion (PCE) [8]. Unfortunately, all these methods are seriously limited due to a rapid growth of the number of training samples necessary to construct the model as a function if increasing parameter space dimensionality.

In this work, the PC-Kriging metamodeling method [9], combining PCE and Kriging, is introduced into the field of antenna design, aiming at fast estimation of the yield at the expense of a possibly small number of EM analyses of the structure at hand. PCE [10] is known to be convenient at capturing the tendency of the objective function, whereas Kriging [11] handles the model response at the training points. PC-Kriging utilizes PCE as the trend function for the Kriging model, supposedly combining the advantages of both metamodels. The PC-Kriging scheme is demonstrated on the Ishigami function and a dual-band patch antenna.

The paper is organized as follows. Formulation of the yield estimation problem is described in Section II. Section III gives the details of the metamodeling methods. The proposed approach is illustrated and compared to the PCE and the Kriging metamodels in Section IV. Section V concludes the work.

II. Antenna Yield Estimiation

Let $\mathbf{R}(\mathbf{x})$ denote the antenna responses of interest evaluated using an EM simulation model, e.g., the reflection characteristic; $\mathbf{x}\in\mathbb{R}^m$ is a vector of designable parameters. The nominal design is denoted by $\mathbf{x}^0 = [\mathbf{x}_1{}^0, \mathbf{x}_2{}^0,\ldots, \mathbf{x}_n{}^0]^T$. Due to the manufacturing tolerances or uncertainties existing in the antenna system, the actual parameters are $\mathbf{x}^0+d\mathbf{x}$, where $d\mathbf{x}$ is a random vector drawn according to a pre-assigned probability distribution.

Let $H(\mathbf{x})$ be a function defined as [1]

$$H(\mathbf{x}) = \begin{cases} 1, & \text{if } \mathbf{R}(\mathbf{x}) \text{ satisfied the design specifications} \\ 0, & \text{otherwise} \end{cases} \quad (1)$$

The yield at the nominal design $\mathbf{x}^0$, i.e., the probability of satisfying the specifications, is given by

$$Y(\mathbf{x}^0) = [\textstyle\sum_{j=1}^{N} H(\mathbf{x}^0 + d\mathbf{x}^j)]/N, \quad (2)$$

where $d\mathbf{x}^j$, j = 1, 2, …, N, are the random deviations as described above.

In this work, for the sake of computational efficiency, the yield is estimated using a response feature approach [1]. This allows us to "flatten" highly nonlinear antenna responses which facilitates construction of the metamodels while being sufficient to determine satisfaction/violation of the design specs.

III. Metamodeling

We start by outlining the two relevant state-of-the-art metamodeling techniques, PCE and Kriging. This puts us in a position do describe the process of constructing a PC-Kriging metamodel.

A. Polynomial Chaos Expansions

Polynomial chaos expansion (PCE) metamodels are generally formulated as [10]

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$$M(\mathbf{x}) = \sum_{i=1}^{\infty} \alpha_i \mathbf{\Psi}_i(\mathbf{x}), \tag{3}$$

where $\mathbf{x} \in \mathbb{R}^m$ is a vector with random independent components described by a probability density function $f_{\mathbf{x}}$, $M(\mathbf{x})$ is a map of the features with respect to $\mathbf{x}$, i is the index of ith polynomial term, $\mathbf{\Psi}_i$ are multivariate polynomial basis functions, whereas α_i are their corresponding expansion coefficient. In practice, a truncated form of the PCE is used

$$M(\mathbf{x}) \approx M^{PC}(\mathbf{x}) = \sum_{i=1}^{P} \alpha_i \mathbf{\Psi}_i(\mathbf{x}), \tag{4}$$

where $M^{PC}(\mathbf{x})$ is the approximate truncated PCE model, and P is the total number of sample points, which can be calculated as

$$P = \frac{(p+n)!}{p!n!}, \tag{5}$$

where p is the order of the PCE, and n is the total number of random input variables.

The coefficient vector $\boldsymbol{\alpha}$ is found by solving a least-squares minimization problem

$$\hat{\boldsymbol{\alpha}} = \arg\min E[\boldsymbol{\alpha}^T \Psi(\mathbf{x}) - M(\mathbf{x})]. \tag{6}$$

In this work, the least-angle regression (LARS) method is used to solve (6) by adding an L_1 penalty term

$$\hat{\boldsymbol{\alpha}} = \arg\min E[\boldsymbol{\alpha}^T \Psi(\mathbf{x}) - M(\mathbf{x})] + \lambda \|\boldsymbol{\alpha}\|_1, \tag{7}$$

where λ is a penalty factor, $\|\boldsymbol{\alpha}\|_1$ is the L_1 norm of the coefficients of PCE.

B. Kriging Interpolation

Kriging interpolation [11], belonging to a class of Gaussian process regression, is an interpolation technique, in which the training points are treated as realizations of the unknown random process. The Kriging coefficients (referred to as hyper-parameters) are found by minimizing the mean square error (MSE). The model is a sum of a low-order polynomial (the trend function) $\mathbf{f}^T(\mathbf{x})\boldsymbol{\beta}$, and a Gaussian deviations $Z(\mathbf{x})$

$$M(\mathbf{x}) = \mathbf{f}^T(\mathbf{x})\boldsymbol{\beta} + Z(\mathbf{x}), \tag{8}$$

where $\mathbf{f}(\mathbf{x}) = [f_0(\mathbf{x}), \ldots, f_{p-1}(\mathbf{x})]^T \in \mathbb{R}^p$ is defined with a set of the regression basis functions, $\boldsymbol{\beta} = [\beta_0(\mathbf{x}), \ldots, \boldsymbol{\beta}_{p-1}(\mathbf{x})]^T \in \mathbb{R}^p$ denotes the vector of the corresponding coefficients, and $Z(\mathbf{x})$ denotes a stationary random process with zero mean, variance and nonzero covariance. In this work, Gaussian exponential correlation function is adopted, thus the nonzero covariance is of the form

$$Cov\left[Z(\mathbf{x}), Z(\mathbf{x}')\right] = \sigma^2 \exp\left[-\sum_{k=1}^{n} \theta_k \left|x_k - x_k'\right|^{p_k}\right], \tag{9}$$

where $\boldsymbol{\theta} = [\theta_1, \theta_2, \ldots, \theta_m]^T$, $\mathbf{p} = [p_1, p_2, \ldots, p_n]^T$, with $1 < p_k \leq 2$, denote the vectors of unknown hyperparameters to be tuned. The Kriging predictor for any untried $\mathbf{x}$ can be written as [8, 9]

$$M^{Kr}(\mathbf{x}) = \mathbf{f}^T(\mathbf{x})\hat{\boldsymbol{\beta}} + \mathbf{r}^T(\mathbf{x})\mathbf{R}^{-1}(\mathbf{M}_S - \mathbf{F}\hat{\boldsymbol{\beta}}), \tag{10}$$

where $\hat{\boldsymbol{\beta}}$ comes from generalized least squares estimation, $\mathbf{r}$ is the correlation vector between $\mathbf{x}$ and training set points, $\mathbf{R}$ is the correlation matrix, $\mathbf{M}_S$ is the model response of the training points, and $\mathbf{F}$ is a matrix of the trend function values at the training points.

C. PC-Kriging

PC-Kriging [9] is a recently developed class of metamodels that integrates PCE and Kriging metamodels. In particular, PCE is utilized as the trend function for the Kriging metamodel. The modeling flow can be described as follows:

1. Obtain observations (training points) from the physics-based simulation model.
2. Generate a PCE model following Section III.A.
3. In Step 2, LARS technique selects the "important" basis terms, meaning those most correlated with the model response.
4. Plug those "important" basis terms into (10), then construct the Kriging model.

IV. Numerical Examples

A. Ishigami Function

The Ishigami function is commonly used to demonstrate modeling under uncertainty, because of its strong nonlinearity and non-monotonicity. The analytical form of the Ishigami function is

$$f(\mathbf{x}) = \sin(x_1) + 7\sin^2(x_2) + 0.1x_3^4\sin(x_1), \tag{11}$$

where x_1, x_2, and x_3 are uniformly distributed on $[-\pi, \pi]$.

Figure 1 shows the root mean squared error (RMSE), as a function of the number of training points. It can be seen that the PC-Kriging metamodel requires around 70 training points, which is over four times fewer training points than the Kriging metamodel in this case, to reach the desired accuracy level. PCE metamodel requires around 75 training points. Here, the PC-Kriging utilizes 10^{th}, 11^{th}, and 12^{th} order PCE as trend function, when provided 60, 65, and 70 training points, respectively.

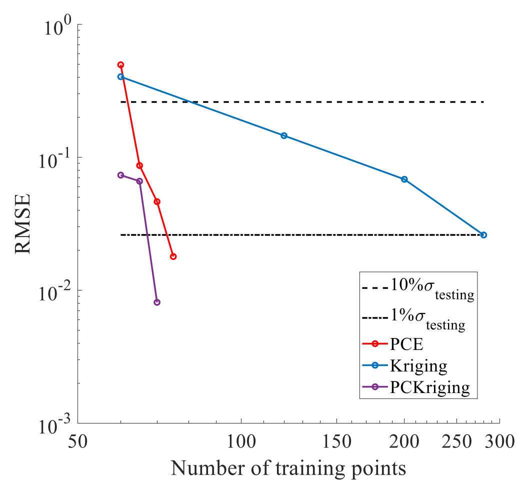

Fig. 1. Metamodel setup for the Ishigami test case.

B. Dual-Band Patch Antenna

Figure 2 shows the geometry of the microstrip dual-band patch antenna used in this work as a benchmark example. The antenna is implemented on a 0.762 mm thick Taconic RF-35 dielectric substrate (ε_r = 3.5). The independent geometry parameters are $\mathbf{x} = [L\ l_1\ l_2\ l_3\ l_4\ W\ w_1\ w_2\ g]^T$. The EM model **R** is implemented in CST. The nominal design, corresponding to the antenna resonances allocated at the frequencies 2.4 GHz and 5.8 GHz is $\mathbf{x}^0 = [14.18\ 3.47\ 12.44\ 5.06\ 15.56\ 0.65\ 8.29\ 5.60]^T$ (all dimensions in mm).

The antenna yield has been estimated for the following specs: $|S_{11}| \le -10$ dB for both 2.4 GHz and 5.8 GHz. Three cases were considered assuming Gaussian distribution of geometry deviation vector $d\mathbf{x}$ with zero mean and variance σ of 0.05 mm. The parametric study on the convergence of the yield value versus the number of training points has been shown in Fig. 3. The PCE, Kriging and PC-Kriging metamodels are compared with the direct Monte Carlo analysis involving 500 EM evaluations of **R**, utilized as a reference.

As shown in Table 1, to reach satisfactory estimations, PCE and Kriging require around 300 and 100 training points, respectively. The proposed PC-Kriging requires only 20 training points, which is a dramatic reduction over both PCE (by a factor of fifteen) and Kriging (by a factor of five).

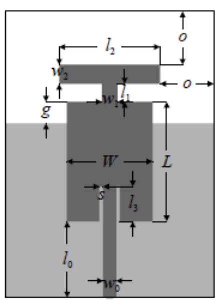

Fig. 2. Geometry of the dual-band patch antenna. Ground plane shown with light gray shade.

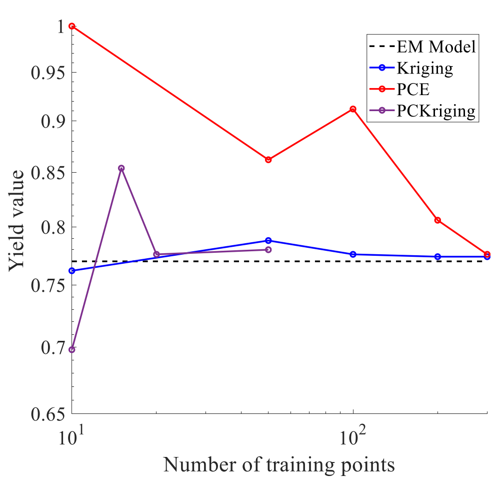

Fig. 3. Convergence of yield estimation as a function of the number of training points for the considered metamodeling techniques as well as direct EM-based Monte Carlo simulation.

Table 1. Computational cost of the yield estimation.

Geometry	Estimation Method	Estimated Yield	Sampling Cost
Gaussian σ = 0.05 mm	EM	0.770	500
	PCE	0.776	300
	Kriging	0.776	100
	PC-Kriging (this work)	0.776	20

V. Conclusion

The PC-Kriging metamodel has been proposed in this work for yield estimation of antennas. The PC-Kriging is constructed as a combination of PCE and Kriging. The former is utilized as a trend function for the latter. The approach was demonstrated on the Ishigami analytical function and a dual-band microstrip patch antenna. The numerical results indicate that PC-Kriging offers considerable reduction of the computational cost of yield estimation as compared to individual metamodels, both PCE and Kriging. Future work will be focused on further characterization of the approach proposed in this paper, especially in terms of its scalability with respect to the parameter space dimension as well as statistical moments of the input probability distribution.

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