Nested Kriging Surrogates for Rapid Multi-Objective Optimization of Compact Microwave Components

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***Abstract*—A procedure for rapid EM-based multi-objective optimization of compact microwave components is presented. Our methodology employs a recently developed nested kriging modelling to identify the search space region containing the Pareto-optimal designs, and to construct a fast surrogate model. The latter permits determination of the initial Pareto set, further refined using a separate surrogate-assisted process. As an illustration, a three-section impedance transformer is designed for the best matching and minimum size. The set of trade-off designs is produced at the low computational cost of only a few hundred of high-fidelity EM simulations of the transformer circuit despite a large number of its geometry parameters.**

Keywords—Microwave optimization, multi-objective design, simulation-driven design, surrogate modelling.

I. INTRODUCTION

Circuit miniaturization has become a common trend in the design of microwave components [1]. Unfortunately, size reduction normally stays in conflict with ensuring desired electrical performance. Finding available design trade-offs can be realized through multi-objective optimization (MO) [2]. MO is a computationally expensive task, because reliable evaluation of compact structures requires full-wave electromagnetic (EM) analysis [3]. At the same time, the most popular MO techniques (population-based metaheuristics, e.g., particle swarm optimizers [4]) are computationally inefficient.

In this paper, a novel technique for MO of compact microwave components is presented, capitalizing on a recently reported nested kriging modeling paradigm [5]. The latter permits identification of the search space region containing the Pareto set and to set up, therein, a fast surrogate further utilized to yield an initial approximation of the trade-off designs. The procedure is supplemented with a surrogate-assisted refinement routine. Despite of using a single-level (high-fidelity) EM model only throughout the process and handling a large number of parameters, our framework is demonstrated to render the Pareto set at a low CPU cost.

II. MULTI-OBJECTIVE DESIGN BY NESTED KRIGING

A goal of MO is to determine a set of globally non-dominated designs representing the best possible trade-offs w.r.t. the objectives F_k, $k = 1, \ldots, N$ [2], all to be minimized. The MO process may be sped up by optimizing directly a faster surrogate model $\boldsymbol{R}_s$, instead of the EM-simulated (fine) model $\boldsymbol{R}(\boldsymbol{x})$ ($\boldsymbol{x}$ denotes the parameter vector), being the primary way of system evaluation. Due to a limited accuracy of the surrogate, the initial Pareto-optimal designs $\boldsymbol{x}_s^{(k)}$ have to be refined as follows:

$$\boldsymbol{x}_f^{(k)} = \arg \min_{\substack{\boldsymbol{x},\, F_2(\boldsymbol{x}) \le F_2(\boldsymbol{x}_s^{(k)}) \\ \vdots \\ F_N(\boldsymbol{x}) \le F_N(\boldsymbol{x}_s^{(k)})}} F_1\left(\boldsymbol{R}_s(\boldsymbol{x}) + [\boldsymbol{R}(\boldsymbol{x}_s^{(k)}) - \boldsymbol{R}_s(\boldsymbol{x}_s^{(k)})]\right), \quad (1)$$

where the last term represents output space mapping correction [7]. In this work, the surrogate is constructed using a recently reported nested kriging modelling approach [5], here, adopted to represent the system responses in the region containing the Pareto set. Let $\boldsymbol{x}^{(j)}$, $j = 1, \ldots, p$, denote the reference designs optimized w.r.t. the performance vectors $\boldsymbol{F}^{(j)} = [F_1^{(j)} \ldots F_N^{(j)}]$, with $\boldsymbol{x}^{(j)} = [x_1^{(j)} \ldots x_n^{(j)}]^T$. The objective space Φ is defined by the ranges $F_{k.\min} \le F_k^{(j)} \le F_{k.\max}$, $k = 1, \ldots, N$. The reference designs need to include the extreme designs $\boldsymbol{x}^{*(k)} = \text{argmin}\{\boldsymbol{x} : F_k(\boldsymbol{R}(\boldsymbol{x}))\}$ (and other designs from the Pareto front if more detailed information is needed). These are obtained by solving:

$$\boldsymbol{x}^{\boldsymbol{w}} = \arg\min_{\boldsymbol{x}} F_1\left(\boldsymbol{R}(\boldsymbol{x})\right), \quad (2)$$

subject to $F_j(\boldsymbol{x}) \le \sum_l w_l F_j(\boldsymbol{x}^{*(l)})$, $j = 2, \ldots, N$; $\boldsymbol{w} = [w_1 \ldots w_N]^T$ is a vector of weights; $0 \le w_j \le 1$ and $\sum_j w_j = 1$. The objective vector $\boldsymbol{F}(\boldsymbol{w})$ refers to the reference design $\boldsymbol{x}^{\boldsymbol{w}}$; $\boldsymbol{w} = [0 \ldots 1 \ldots 0]^T$ (with 1 on the k-th position) corresponds to a single-objective design $\boldsymbol{x}^{*(k)}$. To handle the objective space region spanned by the reference designs an auxiliary mapping h_0 from a unit $N-1$ simplex $S^{N-1} = \{\boldsymbol{z} = [z_1 \ldots z_{N-1}]^T : 0 \le z_k \le 1 \text{ and } \sum_{k=1,\ldots,N-1} z_k \le 1\}$ onto the space of the weights $\boldsymbol{w}$ is used. If $N = 2$ (the case considered in the paper), the mapping h_0 is defined as (generalization for $N > 2$ is straightforward):

$$h_0(\boldsymbol{z}) = \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \begin{bmatrix} -1 & -1 \\ 1 & 0 \end{bmatrix} \cdot \boldsymbol{z}\,. \quad (3)$$

Fig. 1 provides a graphical illustration of the above concepts for $N = 2$. The nested kriging model is to be established in the marked part of the objective space. As the number of available reference designs is in practice limited, these designs merely approximate the Pareto front geometry. Hence, a certain extension is necessary. The extended region O is defined as the set of all points $\boldsymbol{w} = h_0(\boldsymbol{z})\cdot(1 + d)$ with $\boldsymbol{z} \in S^{N-1}$ and $-d_w \le d \le d_w$, where d_w is the extension factor (here, $d_w = 0.05$ is used).

The actual modelling procedure involves two surrogates. The first-level model $\boldsymbol{s}_I(\Phi) \subset X$ (kriging model [6]; with $\{\boldsymbol{F}^{(j)},\boldsymbol{x}^{(j)}\}$ being the training points) maps Φ into the design space X, and it is the first approximation of the surrogate model domain. The $\boldsymbol{s}_I(\Phi)$ is then orthogonally extended towards its normal vectors [5] $\boldsymbol{v}_n^{(k)}(\boldsymbol{F})$, $k = 1, \ldots, n - N$, to ensure that all designs optimal w.r.t. F_k, are comprised in the model domain. Let us define: $\boldsymbol{x}_{\max} = \max\{\boldsymbol{x}^{(k)}, k = 1, \ldots, p\}$, $\boldsymbol{x}_{\min} = \min\{\boldsymbol{x}^{(k)}, k = 1, \ldots, p\}$, $\boldsymbol{x}_d = \boldsymbol{x}_{\max} - \boldsymbol{x}_{\min}$, along with the extension coefficients:

$$\boldsymbol{\alpha}(\boldsymbol{F}) = \left[\alpha_k(\boldsymbol{F})\right]_{k=1,\ldots,n-N}^T = 0.5\tau\left[\,|\,\boldsymbol{x}_d \boldsymbol{v}_n^{(k)}(\boldsymbol{F})\,|\,\right]_{k=1,\ldots,n-N}^T, \quad (4)$$

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where τ is a user-defined thickness parameter. The surrogate model domain X_S is located between the manifolds M_+ and M_-, determined by the coefficients α_k:

$$M_{\pm} = \left\{ \boldsymbol{x} \in X : \boldsymbol{x} = \boldsymbol{s}_I(\boldsymbol{F}) \pm \sum_{k=1}^{n-N} \alpha_k(\boldsymbol{F}) \boldsymbol{v}_n^{(k)}(\boldsymbol{F}) \right\}. \quad (5)$$

Using (5), we define X_S as (cf. [5]):

$$X_S = \left\{ \begin{array}{l} \boldsymbol{x} = \boldsymbol{s}_I(\boldsymbol{F}) + \sum_{k=1}^{n-N} \lambda_k \alpha_k(\boldsymbol{F}) \boldsymbol{v}_n^{(k)}(\boldsymbol{F}) : F \in \Phi, \\ -1 \le \lambda_k \le 1, k = 1,...,n-N \end{array} \right\}. \quad (6)$$

The first-level surrogate comprises two transformations: (i) the mapping h_0 from the Cartesian product of $S^{N-1} \times [-d_w, d_w]$ onto the objective space region O and (ii) the mapping $\boldsymbol{s}_I$ from O into X (merely used for the sake of convenience, as it is easier to implement uniform data sampling on $S^{N-1} \times [-d_w, d_w]$ rather than directly on O). The second-level surrogate is then set up in the orthogonally extended domain $\boldsymbol{s}_I(O)$.

III. Verification Examples

The optimization framework is illustrated using a CMRC-based three-section transformer [7] of Fig. 2, implemented on Taconic RF-35 substrate ($\varepsilon_r = 3.5$, $h = 0.762$ mm), and described by the parameters $\boldsymbol{x} = [l_{1.1}\ l_{1.2}\ w_{1.1}\ w_{1.2}\ w_{1.0}\ l_{2.1}\ l_{2.2}\ w_{2.1}\ w_{2.2}\ w_{2.0}\ l_{3.1}\ l_{3.2}\ w_{3.1}\ w_{3.2}\ w_{3.0}]^T$. The operating range is 1.75 GHz to 4.25 GHz. The figures of interest are: minimization of the in-band reflection (F_1) and minimization of the footprint area (F_2). The computational model $\boldsymbol{R}$ is simulated in CST Microwave Studio (~280,000 mesh cells, simulation time 2.5 min). Four reference designs are used, corresponding to the two single-objective designs and two more for $\boldsymbol{z} = 0.33$ and $\boldsymbol{z} = 0.66$ (cf. (3)).

The nested kriging surrogate was set using only 200 data samples. Its average RMS error is only 4.1%. For comparison, the surrogate was constructed within the reduced interval $\boldsymbol{l}^* = \min\{\boldsymbol{x}^{*(1)}, \boldsymbol{x}^{*(2)}\}$ and $\boldsymbol{u}^* = \max\{\boldsymbol{x}^{*(1)}, \boldsymbol{x}^{*(2)}\}$, typically containing the vast majority of the Pareto front [2]. Although 1600 training samples were used, the model error is 10.4%. The initial Pareto set was obtained by multi-objective evolutionary algorithm (MOEA) [7]. The selected Pareto-optimal designs, before and after refinement are shown in Fig. 3 (a). The reflection characteristics for the selected designs are presented in Fig. 3 (b). Table I contains the breakdown of the optimization cost. The presented approach offers several advantages: (i) the optimization cost, mostly incurred by training data acquisition for setting up the surrogate model, is considerably reduced (by around 65 percent), (ii) the overall MO cost is just 745 EM simulations, and (iii) more precise identification of the initial Pareto set can be obtained (owing to a considerably smaller domain of the nested kriging model and better predictive power of the surrogate).

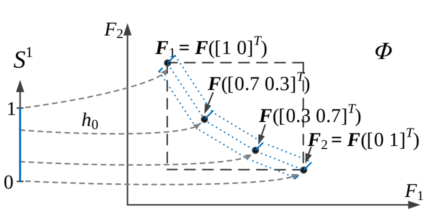

Fig. 1. Objective space Φ and the objective vectors representing selected reference designs; the region of the objective space for setting up the second-level model is marked using dotted lines; the mapping h_0 maps the unity simplex onto the relevant portion of the objective space region (two-objective case).

Fig. 2. CMRC-based three-section impedance matching transformer: (a) compact microstrip resonant cell (CMRC) cell; and (b) transformer geometry.

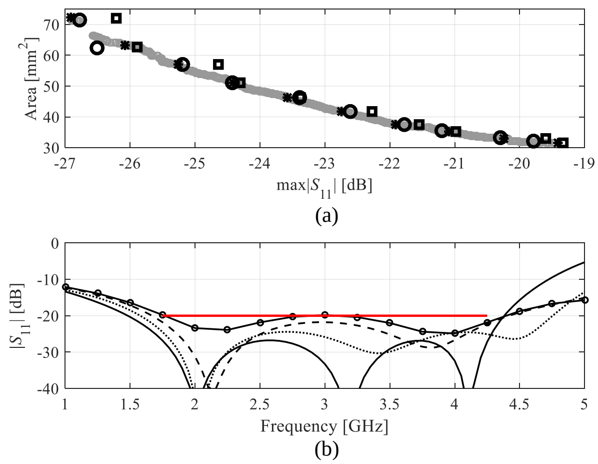

Fig. 3. (a) Pareto-optimal solutions: (o) initial set obtained with MOEA, (*) selected designs for refinement, (□) EM-simulated selected designs, (O) EM-simulated refined designs; (b) reflection characteristics of the transformer for selected Pareto-optimal designs.

TABLE I. Optimization Cost Breakdown

Cost Item	Surrogate Model Domain	
	X_S (this work)	Hypercube $[\boldsymbol{l}^*, \boldsymbol{u}^*]$
Extreme points	$515 \times \boldsymbol{R}$	$515 \times \boldsymbol{R}$
Data acquisition for kriging surrogate	$200 \times \boldsymbol{R}$	$1600 \times \boldsymbol{R}$
MOEA optimization*	N/A	N/A
Refinement	$30 \times \boldsymbol{R}$	$30 \times \boldsymbol{R}$
Total cost#	$745 \times \boldsymbol{R}$ (31 h)	$2145 \times \boldsymbol{R}$ (89 h)

* The cost of MOEA optimization is negligible compared to other stages of the process.
# The total cost (equivalent number of EM simulations; CPU time shown in brackets).

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