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Quality assessment of coarse models and surrogates for space mapping optimization

Slawomir Koziel · John W. Bandler · Kaj Madsen

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Abstract One of the central issues in space mapping optimization is the quality of the underlying coarse models and surrogates. Whether a coarse model is sufficiently similar to the fine model may be critical to the performance of the space mapping optimization algorithm and a poor coarse model may result in lack of convergence. Although similarity requirements can be expressed with proper analytical conditions, it is difficult to verify such conditions beforehand for real-world engineering optimization problems. In this paper, we provide methods of assessing the quality of coarse/surrogate models. These methods can be used to predict whether a given model might be successfully used in space mapping optimization, to compare the quality of different coarse models, or to choose the proper type of space mapping which would be suitable to a given engineering design problem. Our quality estimation methods are derived from convergence results for space mapping algorithms. We provide illustrations and several practical application examples.

Keywords Space mapping · Surrogate modeling · Space mapping optimization · Engineering design optimization · Convergence conditions · Coarse model quality

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S. Koziel (✉)
Simulation Optimization Systems Research Laboratory, Department of Electrical and Computer Engineering, McMaster University, Hamilton, ON, L8S 4K1, Canada
e-mail: koziels@mcmaster.ca

J.W. Bandler
Bandler Corporation, Dundas, ON, L9H 5E7, Canada
e-mail: bandler@mcmaster.ca

K. Madsen
Informatics and Mathematical Modelling, Technical University of Denmark, DK-2800 Lyngby, Denmark
e-mail: km@imm.dtu.dk

1 Introduction

Engineers have used optimization techniques for device and system modeling and design for decades (Steer et al. 2002). Traditional techniques (Bandler and Chen 1988) utilize simulations of appropriate models of the devices and any available derivatives to force relevant system responses to satisfy specifications. For high-fidelity models the cost of application of direct optimization can, however, be prohibitive. Methodologies based on exploitation of iteratively refined surrogates of accurate or high-fidelity models address this issue. Space mapping (Bandler et al. 1994; Bandler et al. 2004d) is an example of this methodology.

There is a rich literature concerning surrogate-based optimization. Alexandrov et al. (2001, 1998) describe the so-called approximation and model management optimization technique. Marsden et al. (2004), Booker et al. (1999), Dennis and Torczon (1997) present a surrogate management framework. Surrogate optimization based on surface response approximation and kriging are discussed in (Leary et al. 2003; Gano et al. 2004). A survey and recommendations for the use of statistical approximation techniques in engineering design are given in (Simpson et al. 2001). Several review papers are available (Barthelemy and Haftka 1993; Torczon and Trosset 1998; Queipo et al. 2005).

In space mapping (SM), the objective function to be optimized is constructed from the responses of a so-called "fine model". By responses, we mean a vector of function values that represents the model's behavior for a given set of design parameter values. It is also assumed that there is an alternative set of functions available, from the so-called "coarse model", not as accurate as those provided by the fine model but much faster to evaluate. SM can link coarse and fine models of different complexities in order to create a surrogate model that is almost as cheap to evaluate as the coarse model and (locally at least) almost as accurate as the fine model.

A number of space mapping algorithms have been developed during the last twelve years, including aggressive space mapping (ASM) (Bandler et al. 2004d), trust-region ASM (Bakr et al. 1998), implicit SM (Bandler et al. 2004a, 2004c), output SM (Bandler et al. 2004b; Koziel et al. 2005), and generalized SM (Koziel et al. 2006). A review and exposition of advances in SM technology is contained in paper (Bandler et al. 2004d). Convergence studies concerning hybrid SM algorithms can be found in (Vicente 2003; Bakr et al. 2001; Madsen and Søndergaard 2004). SM technology is recognized as a contribution to engineering design, especially in the microwave and RF arena (Ros et al. 2005; Rautio 2004; Encica et al. 2005), civil engineering (Pedersen et al. 2005), and structural optimization (Leary et al. 2001; Redhe and Nilsson 2004).

One of the most important issues in space mapping optimization is the quality of the coarse model used in the optimization process, as well as a proper choice of the space mapping type used to construct a surrogate model. Whether or not the coarse model is sufficiently similar to the fine model may be critical to the performance of the space mapping algorithm, and a poor coarse model may result in lack of convergence. On the other hand, the variety of available space mapping types makes it difficult to choose a combination that would be suitable to a given problem in terms of ensuring SM algorithm convergence. Although both the similarity between the coarse and fine models and the quality of the surrogate model can be formulated using proper analytical conditions, it is difficult to verify such conditions beforehand for real-world engineering optimization problems. In this paper, we provide methods of assessing the quality of the coarse model that can be used to predict whether a given model might be successfully used in space mapping optimization, to compare the quality of different coarse models, or to choose the proper type of space mapping which would suit a given optimization problem. Our quality estimation methods are derived from convergence results for space mapping algorithms which are formulated in this paper.

2 Basics of space mapping optimization

Let $f : \Omega_f \to \mathbb{R}^m$, $\Omega_f \subseteq \mathbb{R}^n$, denote the fine model of the engineering device. Our goal is to solve the problem

$$x_f^* \in \arg\min_{x \in \Omega_f} H(f(x)) \tag{1}$$

where $H : \mathbb{R}^m \to \mathbb{R}$ is a given merit function, e.g., a norm. $H \circ f$ is the objective function. We shall denote by Ω_f^* the set of solutions to (1) and call it the set of fine model minimizers.

Definition 1 If Ω_f^* is not empty, we define $H_{\min}$ as $H_{\min} = \min_{x \in \Omega_f} H(f(x))$.

By definition, $H(f(x^*)) = H_{\min}$ if and only if $x^* \in \Omega_f^*$.

We consider the fine model to be expensive to compute and solving (1) by direct optimization to be impractical. Instead, we use surrogate models, i.e., models that are not as accurate as the fine model but are computationally cheap, hence suitable for iterative optimization. We consider a general optimization algorithm that generates a sequence of points $x^{(i)} \in \Omega_f$, $i = 1, 2, \ldots$, and a family of surrogate models $s^{(i)} : \Omega_s^{(i)} \to \mathbb{R}^m$, $i = 0, 1, \ldots$, so that

$$x^{(i+1)} \in \arg\min_{x \in \Omega_f \cap \Omega_s^{(i)}} H(s^{(i)}(x)). \tag{2}$$

If the solution to (2) is non-unique we may impose regularization.

SM assumes the existence of a so-called coarse model $c : \Omega_c \to \mathbb{R}^m$, $\Omega_c \subseteq \mathbb{R}^n$, that describes the same object as the fine model: less accurate but much faster to evaluate. The family of surrogate models is constructed from the coarse model in such a way that $s^{(i)}$ is a suitable distortion of c, such that given matching conditions are satisfied.

Let $\bar{s} : \Omega_s \to \mathbb{R}^m$ be a generic space mapping surrogate model which is the coarse model composed with some suitable space mapping transformations, where $\Omega_s \subseteq \Omega_c \times \Omega_p$, with Ω_p being the parameter space of these transformations. We call Ω_p a space mapping parameter domain. The surrogate model $s^{(i)}$ is defined as

$$s^{(i)}(x) = \bar{s}(x, p^{(i)}) \tag{3}$$

where

$$p^{(i)} \in \arg \min_{p \in \Omega_p^{(i)}} \left(\sum_{k=0}^{i} w_{i.k} \| f(x^{(k)}) - \bar{s}(x^{(k)}, p) \| \right) \tag{4}$$

where $\Omega_p^{(i)} = \{p \in \Omega_p : (x^{(k)}, p) \in \Omega_s \text{ for } k = 0, 1, \dots, i\}$ and $w_{i.k}$ are weighting factors. Typically we use $w_{i.k} = 1$ for $k = 0, 1, \dots, i$. The domain $\Omega_s^{(i)}$ of the surrogate model $s^{(i)}$ is $\Omega_s^{(i)} = \{x \in \Omega_c : (x, p^{(i)}) \in \Omega_s\}$.

As an example, consider the so-called input space mapping (Bandler et al. 1994), in which space mapping is an affine transformation of the coarse model domain of the form $x \to B \cdot x + q$. In this case the generic space mapping surrogate model takes the following form.

$$\bar{s}(x, p) = \bar{s}(x, B, q) = c(B \cdot x + q). \tag{5}$$

Other space mapping types can be found, e.g., in (Koziel et al. 2006).

It is easy to notice that the space mapping algorithm (2–4) has the following two features. First of all, consistency conditions between the fine and surrogate models are not necessarily satisfied. In particular, we do not require that the surrogate model matches the fine model with respect to value and first-order derivative at any of the iteration points. Second, subsequent iterations are accepted regardless of the objective function improvement. As a consequence, convergence of the SM algorithm is not guaranteed in general, and the choice of optimal space mapping approach for a given problem is not obvious. In the next section we will provide methods for assessing the quality of the coarse/surrogate model, which are based on information obtained from the fine model at a set of test points. This information is used to estimate certain conditions in the convergence results and allows us to predict whether a given model might be successfully used in space mapping optimization. Using our method one can also compare the quality of different coarse models, or choose the proper type of space mapping which would suit a given optimization problem.

3 Quality assessment of coarse and surrogate models

We consider the general space mapping surrogate model (3). We assume for simplicity that $\Omega_f = \Omega_c = \Omega$. We start from assumptions concerning the fine and coarse models and then formulate the convergence theorem.

Assumption 1 Suppose that the following conditions are satisfied.

(i) Ω and Ω_p are closed sets.

(ii) Let $\Omega_s^*(p)$ denote a set of solutions to the problem $x_s^* \in \arg\min_{x \in \Omega}\{H(\bar{s}(x, p)) : (x, p) \in \Omega_s\}$. We assume that $\Omega_s^*(p)$ is not empty for any $p \in \Omega_{p.s} = \{r \in \Omega_p : \exists_{x \in \Omega} (x, r) \in \Omega_s\}$ and the following condition is satisfied

$$\sup_{\mathbf{x} \in \Omega_s^*(p)} \sup_{y \in \Omega_s^*(r)} \|x - y\| \le K(r)\|p - r\| \tag{6}$$

for any $p, r \in \Omega_{p.s}$, where $K : \Omega_{p.s} \to \mathbb{R}_+$ is a bounded function on $\Omega_{p.s}$.

(iii) Let $\Omega_p^*(x)$ denote a set of solutions to the surrogate model parameter extraction problem. We assume that $\Omega_p^*(x)$ is not empty. We also assume that there is $k > 1$ such that for each $i > k$, any $p^{(i)} \in \Omega_p^*(x^{(i)})$ and any $p^{(i+1)} \in \Omega_p^*(x^{(i+1)})$ there exist $M_i > 0$ such that

$$\|p^{(i+1)} - p^{(i)}\| \le M_i \|x^{(i+1)} - x^{(i)}\| \tag{7}$$

where $\{x^{(i)}\}$ is the sequence produced by algorithm (2–4).

Assumption 1(ii) requires that the surrogate model optimal solution is regular with respect to the space mapping parameters. Assumption 1(iii) can be easily satisfied in practice if $w_{i.j} > 0$ for all i and j in the parameter extraction process (4), so that the uniqueness of the parameter extraction process is ensured for sufficiently large i.

Having the assumptions we can formulate the following convergence result.

Theorem 1 *Let* $\{(x^{(i)}, p^{(i)})\}$ *be a sequence defined by algorithm* (2–4). *Suppose that Assumption* 1 *is satisfied and for each* $i > k$ *with* k *as in Assumption* 1(iii) *we have*

$$q_i = K(p^{(i)}) \cdot M_i < 1 - \varepsilon \tag{8}$$

where $\varepsilon \in (0, 1)$ *is a small constant independent of* i. *Then, the sequence* $\{x^{(i)}\}$ *is convergent to* x^*, *where* $x^* \in \Omega$ *and the sequence* $\{p^{(i)}\}$ *is convergent to* p^*, *where* $p^* \in \Omega_p$.

Proof Let us take any $x^{(0)} \in \Omega$. Define the sequence $\{x^{(i)}\}$ as in (2), i.e., $x^{(i+1)} \in \arg\min_{x\in\Omega} H(s^{(i)}(x))$ for $i = 1, 2, \ldots$. We need an estimate for $\|x^{(i+2)} - x^{(i+1)}\|$. From Assumption 1(ii) we have

$$\|x^{(i+2)} - x^{(i+1)}\| \le K(p^{(i)})\|p^{(i+1)} - p^{(i)}\|. \tag{9}$$

It follows from (9) and Assumption 1(iii) that, for $i > k$, we have the following estimate.

$$\|x^{(i+2)} - x^{(i+1)}\| \le K(p^{(i)}) \cdot M_i\|x^{(i+1)} - x^{(i)}\| \le q_i\|x^{(i+1)} - x^{(i)}\| \tag{10}$$

with $q_i < 1 - \varepsilon$ for each $i = 1, 2, \ldots$. Now, for any $j > i$ we have

$$\begin{aligned}
\|x^{(j)} - x^{(i)}\| &\le \|x^{(i+1)} - x^{(i)}\| + \|x^{(i+2)} - x^{(i+1)}\| + \cdots + \|x^{(j)} - x^{(j-1)}\| \\
&\le (1 + q_i + q_iq_{i+1} + \cdots + q_iq_{i+1} \cdot \cdots \cdot q_{j-1}q_{j-2}) \cdot \|x^{(i+1)} - x^{(i)}\| \\
&\le (1 + (1-\varepsilon) + (1-\varepsilon)^2 + \cdots + (1-\varepsilon)^{j-i-1}) \cdot \|x^{(i+1)} - x^{(i)}\| \\
&\le \frac{1-(1-\varepsilon)^{j-i}}{1-(1-\varepsilon)}\|x^{(i+1)} - x^{(i)}\| \le \frac{(1-\varepsilon)^{i+1}}{\varepsilon}\|x^{(1)} - x^{(0)}\|
\end{aligned} \tag{11}$$

which is arbitrarily small for sufficiently large i, i.e., $\{x^{(i)}\}$ is a Cauchy sequence. Thus, since Ω is closed, there exists $x^* \in \Omega$, $x^* = \lim_{i\to\infty} x^{(i)}$. Existence of the limit point p^* of the sequence $\{p^{(i)}\}$ can be shown in a similar way. This ends the proof of the theorem. □

Assumption 2 Suppose that Assumption 1 and the following conditions are satisfied.

(i) For any $p \in \Omega_{p.s}$ there is $x \in \Omega$ such that $(x, p) \in \Omega_s$ and $H(\bar{s}(x, p)) \leq H_{\min}$, where $H_{\min}$ is defined in Definition 1.
(ii) Let (x^*, p^*) be a limit point of the sequence $\{(x^{(i)}, p^{(i)})\}$ as in Theorem 1 and $f(x^*) - \bar{s}(x^*, p^*) = 0$ (i.e., the parameter extraction error is zero at the limit point).

Remark 1 Assumption 2(i) is satisfied, in particular, if for any p, $f(\Omega) \subseteq \bar{s}(\{(x, q) \in \Omega_s : q = p\})$.

Corollary 1 *Suppose that Assumption 2 is satisfied, Ω_f^* is not empty, and c, H are continuous. Then $x^* \in \Omega_f^*$, i.e., x^* is an optimal solution of the fine model defined by* (1).

Proof Convergence of the sequence $\{x^{(i)}\}$ follows from Theorem 1. Let $x^* \in \Omega$ be the limit point of $\{x^{(i)}\}$, i.e., $x^* = \lim_{i\to\infty} x^{(i)}$. From Assumption 1 we have $H(\bar{s}(x^{(i+1)}, p^{(i)})) \leq H_{\min}$ for all $i = 0, 1, 2, \ldots$. In particular, we have

$$H_{\min} = \min_{x\in\Omega} H(f(x)) \leq H(f(x^*)) = H(\bar{s}(x^*, p^*)) \leq H_{\min} \tag{12}$$

which gives $x^* \in \Omega_f^*$. The second equality in (12) follows from Assumption 2(ii). The corollary is proved. □

It is seen that for given fine and coarse models, Assumptions 1 and 2 are not easily verified unless both f and c are relatively simple explicit functions. Nevertheless, Theorem 1 and Corollary 1 can be used to derive a simple assessment that would verify whether a given surrogate (i.e., the coarse model enhanced by some space mapping) is likely to assure convergence of the space mapping algorithm. This is important because, as mentioned in the previous section, convergence of the algorithm is not guaranteed in general and algorithm performance depends on the right choice of the coarse model and space mapping type.

We will define a set of quality coefficients that, based on the fine and coarse model data gathered for a set of test points, provide estimates for the product of the bounding function K and numbers M_i, and estimates for the objective function value attainable by the optimized surrogate model as well as estimates for the parameter extraction error. These will allow us to predict whether Assumptions 1 and 2 are likely to be satisfied for a given combination of a coarse model and space mapping. As a result, we can choose the surrogate model that is going to perform well while used in a space mapping algorithm for a given optimization problem.

Let $X_T = \{x_t^{(1)}, x_t^{(2)}, \ldots, x_t^{(N_t)}\} \subset \Omega$ be a set of N_t test points. Let us define the quality factors L_{SM}, H_{SM}, and D_{SM} as follows

$$L_{\mathrm{SM}} = \max_{i,j\in\{1,\ldots,N_t\}, i\neq j} l_{\mathrm{SM}.ij}, \tag{13}$$

$$H_{\mathrm{SM}} = \frac{1}{N_t} \sum_{j=1}^{N_t} H(\bar{s}(y_t^{(j)}, p_t^{(j)})), \tag{14}$$

$$D_{\mathrm{SM}} = \frac{1}{N_t} \sum_{j=1}^{N_t} \| f(x_t^{(j)}) - \bar{s}(x_t^{(j)}, p_t^{(j)}) \| \tag{15}$$

where

$$l_{\mathrm{SM}.ij} = \frac{\| y_t^{(i)} - y_t^{(j)} \|}{\| x_t^{(i)} - x_t^{(j)} \|} \tag{16}$$

and $p_t^{(i)} \in \arg\min_{p \in \Omega_{p.t}} (\sum_{j=1}^{N_t} w_j^{(i)} \| f(x_t^{(j)}) - \bar{s}(x_t^{(j)}, p) \|)$ with $\Omega_{p.t}$ being the domain of the SM parameters corresponding to the current test set, $\Omega_{p.t} = \{p \in \Omega_p : (x_t^{(j)}, p) \in \Omega_s \text{ for } j = 1, \ldots, N_t\}$, and $y_t^{(j)} \in \Omega_s^*(p_t^{(j)})$ being the optimal solution of the SM surrogate obtained with our optimization routine. The weighting factors $w^{(i)}$ should correspond to the distribution of weights used in the actual algorithm. For example, if the SM algorithm uses $w_{i.i} = 1$, $w_{i.k} = 0$ for $k = 0, 1, \ldots, i-1$ (i.e., only the fine model data at the most recent point is used in the parameter extraction process), the weighting factors $w^{(i)}$ should be $w_j^{(i)} = 1$ for $j = i$, and $w_j^{(i)} = 0$ for $j \neq i$. For other weighting schemes we recommend: $w_j^{(i)} = 1$ for $j = i$, and $w_j^{(i)} = \alpha$ for $j \neq i$, with α defined as

$$\alpha = \frac{\beta}{N_t - \beta(N_t - 1)} \tag{17}$$

where

$$\beta = \frac{\sum_{j=0}^{\lceil N_{\max}/2 \rceil - 1} w_{\lceil N_{\max}/2 \rceil . j}}{\sum_{j=0}^{\lceil N_{\max}/2 \rceil} w_{\lceil N_{\max}/2 \rceil . j}} \tag{18}$$

and $N_{\max}$ is the expected maximum number of iterations of the SM algorithm. This definition assures us that the relative effect of increasing $w_j^{(i)}$ from α to 1 in the parameter extraction is the same as that of adding a next iteration point in the middle of the SM algorithm execution (i.e., at iteration $\lceil N_{\max}/2 \rceil$) while using the weighting scheme w.

The quality factor L_{SM} is an estimate of the products $K \cdot M_i$ mentioned in Theorem 1, which determines the convergence properties of the SM algorithm. H_{SM} is an estimate for satisfying Assumption 2. D_{SM} is the measure of the matching error of the surrogate model. D_{SM} can be treated as another measure of confidence for H_{SM} because a large matching error means that the estimation of the objective function value given by H_{SM} cannot be trusted. The number of test points should be chosen so that one can get a good assessment of the surrogate model with reasonable computational cost.

Obviously, the larger the number of test points, the better the estimates we can get, however, in practice, only a few points can provide us with accuracy which is sufficient for practical assessment of the coarse model. If the value of L_{SM} is smaller than 1 it is likely that the space mapping algorithm will converge with a given coarse model, however even with values larger than 1, convergence is not excluded because Theorem 1 is concerned with sufficient conditions only. On the other hand, convergence of the algorithm and convergence to the optimal solution of the fine model are two different issues, which are basically not related to each other, as seen in Theorem 1 and Corollary 1. This is a characteristic feature of space mapping. That is why we define both H_{SM} and D_{SM} as an estimate for the quality of the solution obtained using SM. Normally, H_{SM} should be compared with $H_{\min}$, which is often not known beforehand. In many cases, however, e.g., when we are dealing with minimax optimization, 0 is a threshold value for the objective function H which distinguishes between solutions that satisfy the design specifications ($H \leq 0$) and those not satisfying the design specifications ($H > 0$). In such cases, H_{SM} should be compared with 0. The value of D_{SM} should be as small as possible. On the other hand, if one wants to compare different coarse models or different space mapping surrogate types, it is enough to directly compare the values of L_{SM}, H_{SM} and D_{SM} corresponding to these models.

It is advisable to choose test points as close to the expected location of the fine model solution as possible, because convergence of the space mapping algorithm is determined by the values of function K and number M_i (see Assumption 1) in the neighborhood of the limit point.

4 Examples

In this section we consider two examples of engineering design optimization problems. Our examples are chosen to illustrate how the assessment methodology described in this paper can help in choosing the proper space mapping surrogate model to solve a given optimization problem. In all numerical experiments, both for space mapping optimization and the direct optimization, the starting point is chosen to be the coarse model optimal solution.

4.1 Second-order tapped-line microstrip filter

Consider the following optimization problem: a second-order tapped-line microstrip filter (Manchec et al. 2006) shown in Fig. 1. The design parameters are $x = [L_1\ g]^T$, where L_1 and g are the length and gap parameters shown in Fig. 1. The fine model f is simulated in FEKO (FEKO® 2004). Evaluation time for the fine model is about 15 minutes on a 3.4 GHz processor. The design specifications are $|S_{21}| \leq -20$ dB for 3.0 GHz$\leq \omega \leq$ 4.0 GHz, $|S_{21}| \geq -3$ dB for 4.75 GHz $\leq \omega \leq$ 5.25 GHz and $|S_{21}| \leq -20$ dB for 6.0 GHz $\leq \omega \leq$ 7.0 GHz, where S_{21} is the complex transmission coefficient between the input and output ports. We use a minimax objective function (Zhu et al. 2007) in this problem. The model response is the evaluation of $|S_{21}|$ at 33 frequency points uniformly distributed in the interval 3 to 7 GHz. The coarse model c is the circuit model implemented in Agilent ADS (Agilent ADS 2003) shown in Fig. 2. Evaluation time for c is a couple of milliseconds. The initial design is the coarse model optimal solution $x^{(0)} = [7.00\ 0.059]^T$ mm. Figure 3 shows the

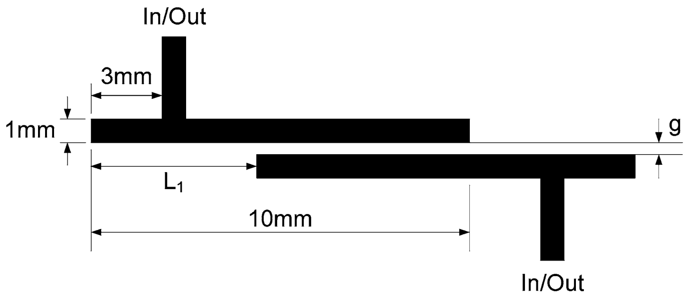

Fig. 1 Geometry of the second-order tapped-line microstrip filter (Manchec et al. 2006)

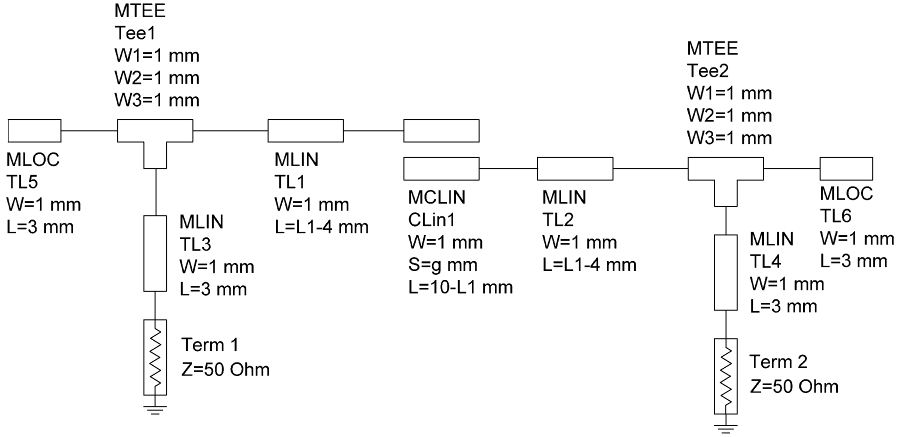

Fig. 2 Coarse model of the second-order tapped-line microstrip filter (Agilent ADS)

Fig. 3 Second-order tapped-line microstrip filter: fine model response (*solid line*) and coarse model response (*dashed line*) at the initial design $x^{(0)}$

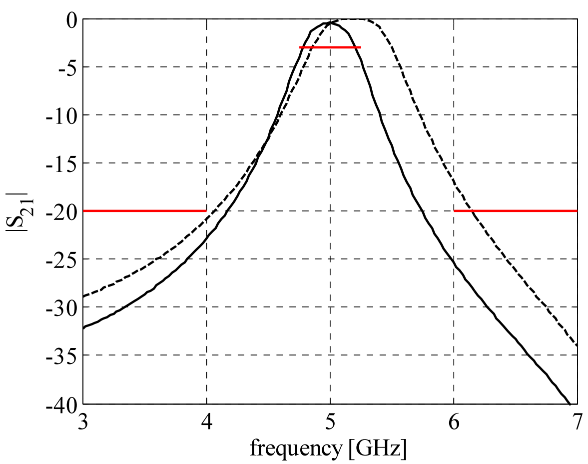

Table 1 Second-order tapped-line microstrip filter: quality factor values and optimization results

Surrogate model	L_{SM}	H_{SM} [dB]	D_{SM}	Objective function value [dB]
$\bar{s}_1$	1.77	0.62	0	−0.40
$\bar{s}_2$	2.17	−0.34	0	−0.21
$\bar{s}_3$	0.37	−0.73	0	−0.72

fine and coarse model response at $x^{(0)}$. Neither the coarse model nor the fine model satisfies the design specifications at the initial design, i.e., the corresponding objective function values are positive.

We use three surrogate models: $\bar{s}_1(x, p) = \bar{s}_1(x, q, d) = c(x + q) + d$, which corresponds to input space mapping and output space mapping; $\bar{s}_2(x, p) = \bar{s}_2(x, p_f, d) = c_f(x, p_f) + d$, which corresponds to frequency and output space mapping, where c_f is a frequency-mapped coarse model, i.e., the coarse model evaluated at frequencies different from the original frequency sweep for the fine model, according to the mapping $\omega \to p_{f.1} + p_{f.2}\omega$, with $p_f = [p_{f.1}\ p_{f.2}]^T$; $\bar{s}_3(x, p) = \bar{s}_3(x, p_i, d) = c_i(x, p_i) + d$, which corresponds to implicit and output space mapping, where c_i is an implicit-space-mapped coarse model with preassigned parameters $p_i = [\varepsilon_r\ H]^T$, where ε_r and H are relative permittivity and thickness of the dielectric substrate of the filter, respectively. In all models, input/frequency/implicit SM parameters are extracted as in (4) with $w_{i.k} = 1$ for $k = 0, 1, \ldots, i$. The output SM parameter d is calculated as $d = f(x) - c(x + q)$ for model $\bar{s}_1, d = f(x) - c_f(x, p_f)$ for model $\bar{s}_2$, and $d = f(x) - c_i(x, p_i)$ for model $\bar{s}_3$ after the extractable SM parameters are known.

For our three surrogate models, we calculate the values of L_{SM}, H_{SM} and D_{SM} using the same set X_T consisting of 5 points: the starting point $x^{(0)}$ and four random points in its neighborhood. Then, we perform optimization using algorithm (2–4). Table 1 shows the values of the quality factors as well as the value of the objective function for all the three coarse models considered. Note that D_{SM} equals zero in all cases by the definitions of the surrogate models. Figure 4 shows the convergence properties for the SM algorithm using all the considered coarse models.

Our results indicate that the performance of the algorithms complies with the prediction obtained using the quality factors L_{SM} and H_{SM}. The value of L_{SM} for the model $\bar{s}_1$ is 1.77, and 2.17 for model $\bar{s}_2$, which indicates convergence problems. Indeed, the plots in Fig. 4 confirm this. In fact, we can observe convergence, which is, however, very slow. L_{SM} for the model $\bar{s}_3$ is much smaller than 1, and the SM algorithm is actually convergent.

Also, the solution found by the algorithm working with model $\bar{s}_3$ is better than the solution found by the algorithm working with models $\bar{s}_1$ and $\bar{s}_2$. Figure 5 shows the fine model response at the solution $x^* = [6.317\ 0.050]^T$ found by the SM algorithm with the surrogate model $\bar{s}_3$.

For comparison purposes we performed direct optimization of the fine model using the Matlab *fminimax* method (Matlab™ 2005) which is based on sequential quadratic programming and line searches. We also performed SM optimization with the surrogate model $\bar{s}_3$ and a warm start of the algorithm in which all the test points used in the

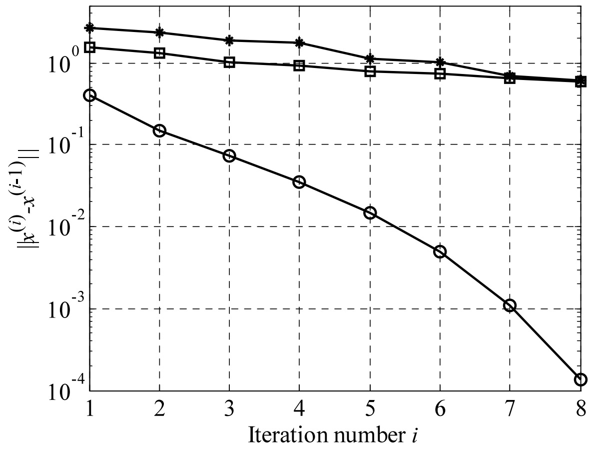

Fig. 4 Second-order tapped-line microstrip filter: convergence properties for the SM algorithm using the surrogate model $\bar{s}_1\,(*)$, $\bar{s}_2$ ($\square$), and $\bar{s}_3\,(\mathrm{o})$

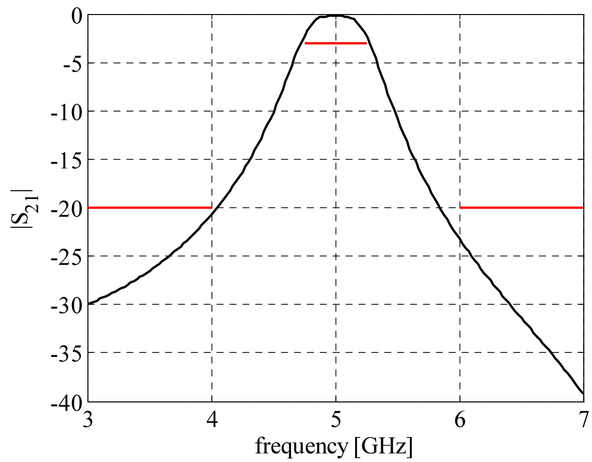

Fig. 5 Second-order tapped-line microstrip filter: fine model response at the solution found by the SM algorithm with the surrogate model $\bar{s}_3$

model assessment are employed to create the initial surrogate model for the SM algorithm. Table 2 compares of the computational complexity of the direct optimization and SM optimization without and with the warm start, as well as the computational effort of the assessment procedure itself. As we can see, the total SM optimization time including surrogate model assessment is substantially smaller than the direct optimization time. The savings is 83%. By reusing the fine model data obtained during the assessment phase we can additionally save two fine model evaluations and reduce the total execution time by 32 minutes. The savings with respect to direct optimization is 86%.

4.2 Microstrip bandpass filter with two transmission zeros

Our second example is a microstrip bandpass filter with two transmission zeros (Hsieh and Chang 2003) shown in Fig. 6. The design parameters are $x = [L_1\ L_2\ g\ s\ d]^T$, where $L_1,\ L_2,\ g,\ s$ and d are geometrical parameters defined in

Table 2 Second-order tapped-line microstrip filter: comparison of computational complexity for direct and space mapping optimization

Procedure	Number of fine model evaluations	Objective function value [dB]	Total execution time*
Direct optimization	83	−0.70	1228 min
Surrogate model assessment	5	N/A	79 min
SM optimization	8	−0.72	124 min
Surrogate model assessment + SM optimization	13		203 min
SM optimization with warm start	6	−0.72	93 min
Surrogate model assessment + SM optimization with warm start	11		172 min

*Total execution time includes the total fine model evaluation time and all the overhead related to parameter extraction and surrogate optimization

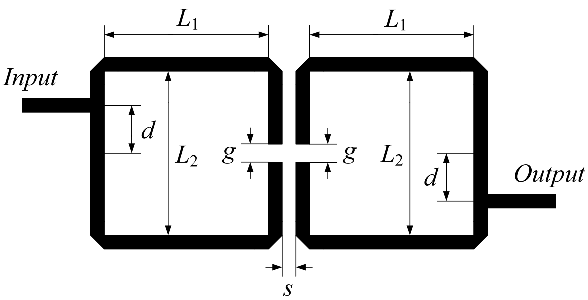

Fig. 6 Geometry of the bandpass filter with two transmission zeros (Hsieh and Chang 2003)

Fig. 6. The fine model f is simulated in FEKO (FEKO® 2004). Evaluation time for the fine model is about 25 minutes on a 3.4 GHz processor. The design specifications are $|S_{21}| \leq -20$ dB for 1.0 GHz $\leq \omega \leq$ 1.7 GHz, $|S_{21}| \geq -3$ dB for 1.9 GHz $\leq \omega \leq$ 2.1 GHz and $|S_{21}| \leq -20$ dB for 2.3 GHz $\leq \omega \leq$ 3.0 GHz. We use a minimax objective function (Zhu et al. 2007). The model response is the evaluation of $|S_{21}|$ at 41 frequency points uniformly distributed in the interval 1 to 3 GHz. The coarse model c is the circuit model implemented in Agilent ADS (Agilent ADS 2003) shown in Fig. 7. Evaluation time for c is several milliseconds. The initial design is the coarse model optimal solution $x^{(0)} = [3.374\ 10.89\ 0.113\ 0.344\ 2.699]^T$ mm. Figure 8 shows the fine and coarse model response at $x^{(0)}$.

We use four surrogate models: $\bar{s}_1(x, p) = \bar{s}_1(x, q) = c(x + q)$, which corresponds to input space mapping; $\bar{s}_2(x, p) = \bar{s}_2(x, q, p_f) = c_f(x + q, p_f)$, which corresponds to input space mapping with c_f being a frequency-mapped coarse model, i.e., the coarse model evaluated at frequencies different from the original frequency sweep for the fine model, according to the mapping $\omega \to p_{f.1} + p_{f.2}\omega$, with $p_f = [p_{f.1}\ p_{f.2}]^T$; $\bar{s}_3(x, p) = \bar{s}_1(x, q, d) = c(x + q) + d$, which corresponds to input and output space mapping; and $\bar{s}_4(x, p) = \bar{s}_2(x, q, p_f, d) = c_f(x + q, p_f) + d$, which corresponds to input and output space mapping with c_f as in $\bar{s}_2$. In all models, the SM parameters

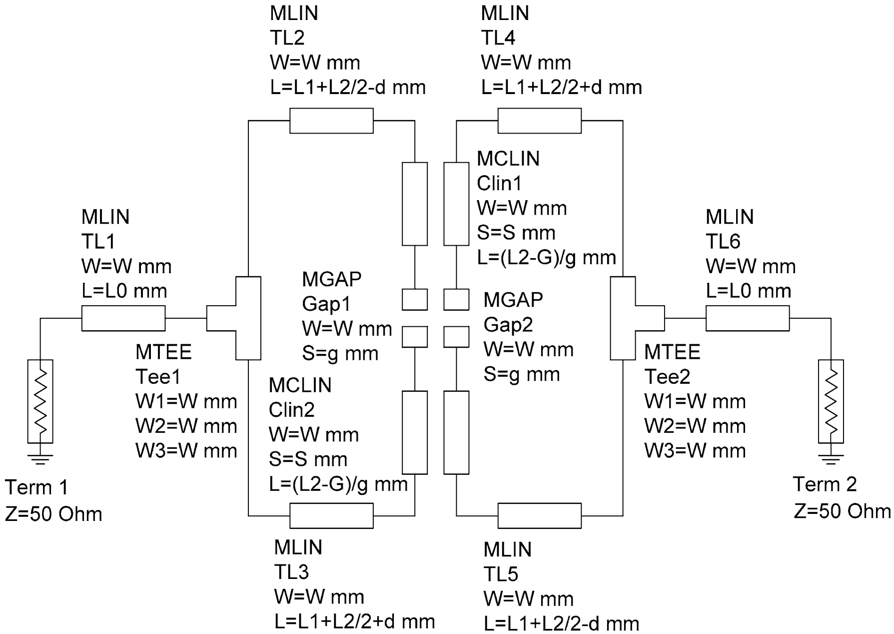

Fig. 7 Coarse model of the bandpass filter with two transmission zeros (Agilent ADS)

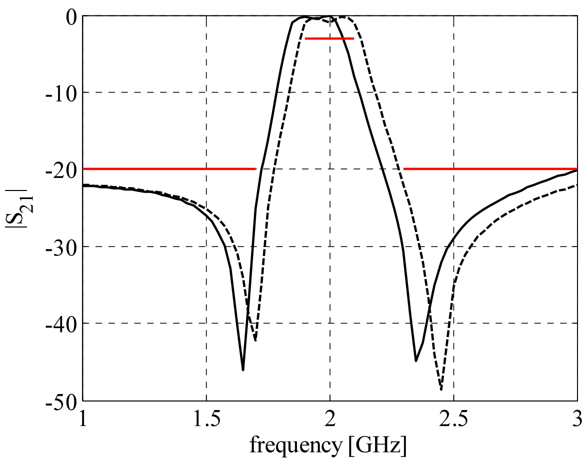

Fig. 8 Bandpass filter with two transmission zeros: fine model response (*solid line*) and coarse model response (*dashed line*) at the initial design $x^{(0)}$

are extracted as in (4) with $w_{i.k} = 1$ for $k = 0, 1, \ldots, i$. The output SM parameter d is calculated as $d = f(x) - c(x + q)$ for model $\bar{s}_3$, and $d = f(x) - c_f(x + q, p_f)$ for model $\bar{s}_4$, after the extractable SM parameters are known.

For all surrogate models, we calculate values of L_{SM}, H_{SM} and D_{SM} using the same set X_T consisting of 5 points: the starting point $x^{(0)}$ and four random points in its neighborhood. Then, we perform optimization using algorithm (2–4). Table 3 shows the values of the quality factors as well as the value of the objective function

Table 3 Bandpass filter with two transmission zeros: quality factor values and optimization results

Surrogate model	L_{SM}	H_{SM} [dB]	D_{SM}	Objective function value [dB]
$\bar{s}_1$	0.17	−2.05	0.022	−1.51
$\bar{s}_2$	0.15	−2.05	0.023	−1.79
$\bar{s}_3$	8.7	−1.57	0	+4.09
$\bar{s}_4$	12.6	−1.92	0	+3.50

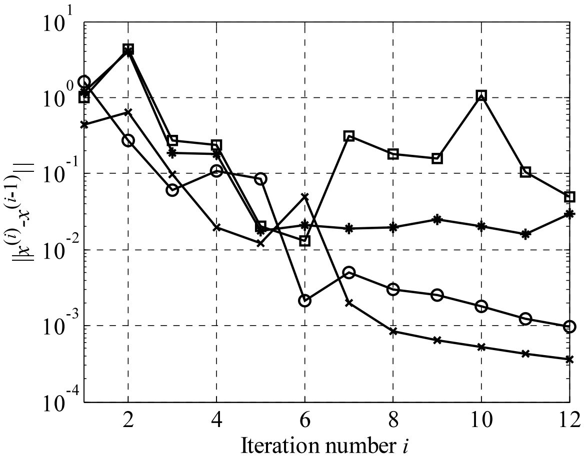

Fig. 9 Bandpass filter with two transmission zeros: convergence properties for the SM algorithm using the surrogate model $\bar{s}_1\,(\times)$, $\bar{s}_2$ (o), $\bar{s}_3$ (□), and $\bar{s}_4$ $(*)$

for all the three coarse models considered. Figure 9 shows the convergence properties for the SM algorithm using all the considered coarse models. Figure 10 shows the fine model response at the solution $x^* = [2.371\ 11.879\ 0.569\ 0.364\ 2.558]^T$ found by the SM algorithm with the surrogate model $\bar{s}_3$.

Based on the values of the quality factors in Table 3 we can predict that the space mapping algorithm using surrogate models that use the output space mapping term d should perform worse than the algorithm working with models not using the output space mapping, which is actually the case, even if the output space mapping allows us to obtain perfect matching between the surrogate and the fine model at the current iteration point (i.e., $D_{SM} = 0$). Note also that D_{SM} for models $\bar{s}_1$ and $\bar{s}_2$ is very small, which means that input and input/frequency space mapping is able to substantially remove the mismatch between the fine and surrogate models.

For comparison purposes we performed direct optimization of the fine model using the Matlab *fminimax* method (Matlab™ 2005). We also performed SM optimization with the surrogate model $\bar{s}_2$ and the warm start of the algorithm in which all the test points used in the model assessment are employed to create the initial surrogate model for the SM algorithm. Table 4 compares of the computational complexity of the direct optimization and SM optimization without and with the warm start as well as the computational effort of the assessment procedure itself. The total SM optimization time including surrogate model assessment is substantially smaller than the direct optimization time. The savings is 93.5%. By reusing the fine model data obtained during the assessment phase we can additionally save three fine model evaluations

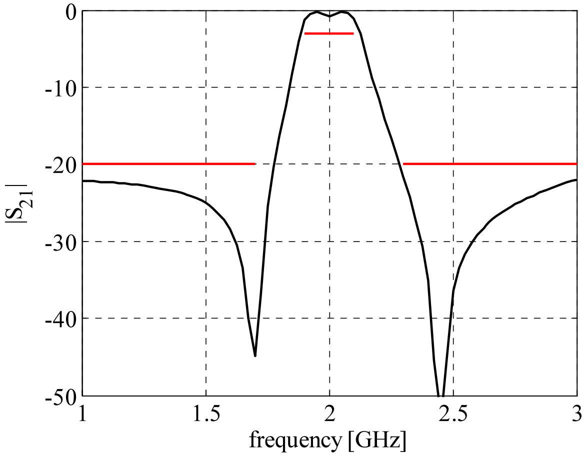

Fig. 10 Bandpass filter with two transmission zeros: fine model response at the solution found by the SM algorithm with the surrogate model $\bar{s}_2$

Table 4 Bandpass filter with two transmission zeros: comparison of computational complexity for direct and space mapping optimization

Procedure	Number of fine model evaluations	Objective function value [dB]	Total execution time*
Direct optimization	245	−1.69	102 hours 3 min
Surrogate model assessment	5	N/A	2 hours 15 min
SM optimization	12	−1.79	5 hours 12 min
Surrogate model assessment + SM optimization	17		7 hours 27 min
SM optimization with warm start	9	−1.58	4 hours 1 min
Surrogate model assessment + SM optimization with warm start	14		6 hours 16 min

*Total execution time includes the total fine model evaluation time and all the overhead related to parameter extraction and surrogate optimization

and reduce the total execution time by 1 hour and 11 minutes. The savings with respect to direct optimization is 94.5%. The value of the objective function is slightly worse though.

5 Conclusions

We have formulated quality factors that allow us to predict the performance of a space mapping optimization algorithm that uses a particular surrogate formulation. These quality factors are derived from convergence results for a general space mapping optimization algorithm. They are based on a set of test points and aim at estimating whether or not a given combination of coarse/fine model and space mapping formulation is likely to satisfy convergence conditions. They can be used to compare different coarse models as well as different space mapping types to suggest a combination that may be suited to a given problem. The examples we have provided illustrate our approach and indicate its usefulness.

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