Articles

Space Mapping for Engineering Optimization[1]

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1. Introduction

Engineers have used optimization techniques for device and system modeling and design for decades [1]. Traditional techniques [2, 3] utilize simulations of appropriate models of the devices and any available derivatives to force relevant system responses to satisfy specifications subject to design constraints. The higher the fidelity (accuracy) of the models the more expensive we expect the application of traditional optimization to be. For complex problems this cost may be prohibitive.

Methodologies based on exploitation of iteratively refined surrogates of accurate or high-fidelity models address this issue. Through the construction of a suitably accurate physics-based surrogate model one can represent the objective function over a region of the design space. Then, instead of optimizing the high-fidelity model, one can optimize the surrogate which is further locally refined as increasingly accurate model data becomes available. Space mapping [4, 5, 6] is an example of this methodology. Such methods are called *surrogate-based* methods as opposed to the *direct* methods mentioned in the first paragraph.

There is a rich literature concerning surrogate-based optimization. Alexandrov *et al.* [7, 8, 9] describe the so-called approximation and model management optimization technique. This assumes that the surrogate model satisfies so-called zero- and first-order consistency conditions with the high-fidelity model in question. Surrogate models based on second-order corrections are described in [10]. Dennis *et al.* [11, 12, 13] and Serafini [14] present a surrogate management framework and applications for engineering design. Surrogate optimization based on surface response approximation and kriging are discussed in [15, 16, 17]. Ong *et al.* [18] present evolutionary optimization via surrogate modeling. A survey and recommendations for the use of statistical approximation techniques in engineering design are given in [19]. Several review papers are available, including [20, 21, 22] and the recent paper [23].

We would like to emphasize that a characteristic feature that differentiates space mapping from several other surrogate-based optimization methods is that in our vision of space mapping, the surrogate model is constructed using an available, low-fidelity (and physically meaningful) model of the object response (the model being a function of the design variables), rather than pure interpolation/approximation. This is in keeping with the engineering tradition of developing for design purposes meaningful (not necessarily complex, often very simple) models of components of the physical world. Indeed, highly complex engineering component and system designs have been built before high-fidelity validations were computationally feasible.

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, and from which any required constraint and objective function values are directly obtained. In the SM technology, conceived by Bandler in 1993, it is also assumed that there is an alternative set

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of functions available, not as accurate as those provided by the fine model but much faster to evaluate. These functions are derived from a so-called "coarse model." When the coarse model incorporates the same physics as the fine model, it is expected to yield its accuracy over a wide region of the parameter space. For example, in the radio-frequency (RF) and microwave area of electrical engineering, full-wave electromagnetic (EM) simulators can serve as fine models. Another example of a fine model is a physical experiment. Low-fidelity EM simulations or empirical electrical equivalent-circuit models could serve as coarse models. There is a vast library of such models in electrical engineering. Without such a library, the elements of which are continually being augmented and refined, electrical power systems, telecommunications circuits and systems, and computers would be literally unimaginable.

It was demonstrated in [4, 5], how SM can intelligently 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) almost as accurate as the fine model. In some engineering cases, the "coarse" model that is selected can even exhibit ideal or idealized behavior. The SM approach, either upfront or on the fly, updates the surrogate to better approximate the corresponding fine model in a region of interest.

In the first-proposed or original algorithm of Bandler *et al.* [4] the so-called coarse model is viewed as an idealization of the engineering device under consideration. As a result its optimal response is taken as the target response, i.e., the desired value of the objective function. The mapping between the parameter spaces of the coarse and fine models is called the space mapping. It maps available data points in the two spaces (i.e., fine and coarse model domains) which provide similar responses. It is evaluated in a process called parameter extraction (PE). In [4] surrogates are built based on linear approximations of the space mapping. Hence, in each iteration, the surrogate is a linearly mapped coarse model. The next iteration point is found as an optimal solution of the current surrogate.

A number of space mapping algorithms have been developed during last ten years, including aggressive space mapping (ASM) [5], trust-region ASM [24], implicit SM [25, 26], and output SM [27, 28, 29]. A review and exposition of advances in SM technology is contained in paper [6]. As we show in this paper, all of the existing space mapping approaches can be viewed as particular cases of one, generic formulation of space mapping.

Bandler *et al.* [6] offers a mathematical motivation, places SM into the context of classical optimization based on local Taylor approximations and provides an extensive review of successful applications in many branches of engineering.

SM technology is recognized as a contribution to engineering design [30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40], especially in the microwave and RF arena. Snel (Philips, The Netherlands) used SM for new library models of RF components [32]. Hong and Lancaster [30] describe the aggressive SM algorithm as an elegant approach to microstrip filter design. Bakr *et al.* [33] employ artificial neural networks and Bandler *et al.* [34] study SM-based model enhancement. Ismail *et al.* [31] (Com Dev, Canada) use SM for the large-scale design of microwave filters and multiplexers for satellite communications. Pedersen *et al.* [35] utilize an output SM-based surrogate for modeling the thermo active components in new buildings. Ros *et al.* [36] use aggressive SM to design inductively coupled rectangular waveguide filters. Rautio [37] uses implicit SM for design of thick, tightly coupled conductors. He validates his model with a spiral inductor on silicon. Encica *et al.* [38] utilize SM to solve a shape optimization problem using Ansoft Maxwell2D. In automobile crashworthiness finite element simulations, each evaluation is expensive. Redhe and Nilsson [40] report that SM reduces the total computing time to optimize a vehicle's structure up to 50% compared with traditional optimization. SM has been applied to the complete finite element model of the new Saab 9-3 Sport Sedan. Intrusion into the passenger compartment area after the impact was reduced by 32% with no reduction in other crashworthiness responses.

Mathematicians are addressing mathematical interpretations of the formulation and convergence issues of SM algorithms [41, 42, 43, 44], although to date, convergence studies concerning SM consider only hybrid algorithms. In these papers, the authors utilized the general methodology of trust regions, made possible by their formulation of the response vector as a convex combination of the mapped coarse model and fine model response vectors. However, the convergence theories heavily rely on the combination with a classical Taylor-based method as a safeguard in the iteration. Therefore, classical principles of convergence proof are feasible. Unfortunately, it is not possible to prove convergence of "genuine" or pure SM algorithms in this way or explain their observed successful practical behavior because we don't necessarily have local model interpolation at the current iterate. Furthermore, tentative iterates may be accepted regardless of the improvement of the objective function (the fine model).

The development of the convergence theory for genuine SM algorithms is currently work in progress. In general, the conditions under which we can guarantee convergence of this class of algorithms concern SM and the engineering optimization problem itself (i.e., the accuracy of the coarse model as an approximation to the fine model). It follows that convergence depends on the quality of the match between the coarse and fine models. The convergence rate is also subject to the same consideration.

2. Optimization Using Surrogate Models

Let us state an engineering design problem as follows. Let $\boldsymbol{R}_f : X_f \to \mathbb{R}^m$ denote the response vector of a fine model of the engineering device, where $X_f \subseteq \mathbb{R}^n$. The vector $\boldsymbol{R}_f$ expresses the performance of the device, typically in terms of a measured output signal. In other words, we refer to "response" as a vector of function values associated with a given device. Our goal is to solve the problem

$$\boldsymbol{x}_f^* = \arg\min_{\boldsymbol{x}\in X_f} U(\boldsymbol{R}_f(\boldsymbol{x})) \tag{1}$$

where $U : \mathbb{R}^m \to \mathbb{R}$ is a given objective function. Note that the mathematical community typically refers to $U \circ \boldsymbol{R}_f$ as the objective function. We shall denote by X_f^* the set of solutions to (1) and call it the set of fine model minimizers.

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 $\boldsymbol{x}^{(i)} \in X_f, i = 1, 2, \ldots,$ and a family of surrogate models $\boldsymbol{R}_s^{(i)} : X_s^{(i)} \to \mathbb{R}^m, i = 0, 1, \ldots,$ so that

$$\boldsymbol{x}^{(i+1)} = \arg \min_{\boldsymbol{x}\in X_f \cap X_s^{(i)}} U(\boldsymbol{R}_s^{(i)}(\boldsymbol{x})) \tag{2}$$

and $\boldsymbol{R}_s^{(i+1)}$ is constructed using suitable matching conditions with the fine model at $\boldsymbol{x}^{(i+1)}$ (and, perhaps, some of the $\boldsymbol{x}^{(k)}, k = 1,\ldots, i$). If the solution to (2) is non-unique we may impose regularization. We may match responses, i.e.,

$$\boldsymbol{R}_s^{(i)}(\boldsymbol{x}^{(i)}) = \boldsymbol{R}_f(\boldsymbol{x}^{(i)}) \tag{3}$$

and/or match first-order derivatives

$$\boldsymbol{J}_{\boldsymbol{R}_s^{(i)}}(\boldsymbol{x}^{(i)}) = \boldsymbol{J}_{\boldsymbol{R}_f}(\boldsymbol{x}^{(i)}) \tag{4}$$

where $\boldsymbol{J}_{\boldsymbol{R}_s^{(i)}}$ and $\boldsymbol{J}_{\boldsymbol{R}_f}$ denote Jacobians of the surrogate and fine models, respectively. More precisely, we try to define models so that conditions such as (3) and (4) are satisfied.

3. SM-Based Surrogate Models

The family of surrogate models $\{\boldsymbol{R}_s^{(i)}\}$ can be implemented in various ways. SM assumes the existence of a so-called coarse model that describes the same object as the fine model: less accurate but much faster to evaluate. It takes advantage of this fact by shifting the optimization burden into the coarse model.

Let $\boldsymbol{R}_c : X_c \to \mathbb{R}^m$ denote the response vectors of the coarse model, where $X_c \subseteq \mathbb{R}^n$. By $\boldsymbol{x}_c^*$ we denote the optimal solution of the coarse model, i.e.,

$$\boldsymbol{x}_c^* = \arg\min_{\boldsymbol{x}\in X_c} U(\boldsymbol{R}_c(\boldsymbol{x})) \tag{5}$$

We denote by X_c^* the set of all $\boldsymbol{x} \in X_c$ satisfying (5) and call it the set of coarse model minimizers. In the SM framework, the family of surrogate models is constructed from the coarse model in such a way that each $\boldsymbol{R}_s^{(i)}$ is a suitable distortion of $\boldsymbol{R}_c$, such that given matching conditions are satisfied. In what follows, we discuss surrogate models that follow from original space mapping, input space mapping, output space mapping (OSM) and implicit space mapping (ISM).

3.1 The Original SM-Based Surrogate Model

The original SM assumes the existence of a mapping $\boldsymbol{P} : X_f \to X_c$ such that $\boldsymbol{R}_c(\boldsymbol{P}(\boldsymbol{x}_f)) \approx \boldsymbol{R}_f(\boldsymbol{x}_f)$ (proximity of $\boldsymbol{R}_c$ and $\boldsymbol{R}_f$ is measured using a suitable metric) on X_f or at least on some subset of X_f which is of our interest. For any given $\boldsymbol{x}_f \in X_f$, $\boldsymbol{P}(\boldsymbol{x}_f)$ is defined using parameter extraction

$$\boldsymbol{P}(\boldsymbol{x}_f) = \arg\min_{\boldsymbol{x}\in X_c} \|\boldsymbol{R}_c(\boldsymbol{x}) - \boldsymbol{R}_f(\boldsymbol{x}_f)\| \qquad (6)$$

This is illustrated in Figure 3.1.

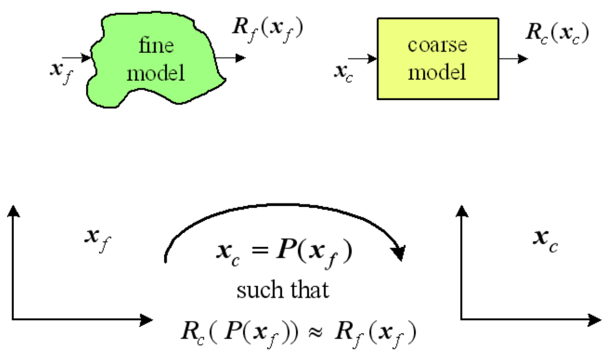

Figure 3.1 Space mapping $\boldsymbol{P}$.

In practical implementation, one may need to use regularization in order to assure existence of the space mapping $\boldsymbol{P}$ (i.e., existence and uniqueness of solution to (6) for any $\boldsymbol{x}_f$). This issue will not be dealt with in the present paper.

The surrogate model $\boldsymbol{R}_s^{(i)}$ is defined as

$$\boldsymbol{R}_s^{(i)}(\boldsymbol{x}) = \boldsymbol{R}_c(\boldsymbol{P}(\boldsymbol{x}^{(i)}) + \boldsymbol{B}^{(i)} \cdot (\boldsymbol{x} - \boldsymbol{x}^{(i)})) \qquad (7)$$

for $i = 0, 1, \ldots,$ where $\boldsymbol{P}$ is defined by (6) and $\boldsymbol{B}^{(i)}$ is an approximation of $\boldsymbol{J}_{\boldsymbol{P}}(\boldsymbol{x}^{(i)})$, the Jacobian of $\boldsymbol{P}$ at $\boldsymbol{x}^{(i)}$, obtained using, e.g., the Broyden formula.

In a practical implementation, e.g., [5], instead of using directly the generic algorithm (2), the next iteration point $\boldsymbol{x}^{(i+1)}$ is obtained as a solution to the equation

$$\boldsymbol{P}(\boldsymbol{x}^{(i)}) + \boldsymbol{B}^{(i)}(\boldsymbol{x}^{(i)}) \cdot (\boldsymbol{x}^{(i+1)} - \boldsymbol{x}^{(i)}) = \bar{\boldsymbol{x}}_c^* \qquad (8)$$

where $\bar{\boldsymbol{x}}_c^*$ is an element of X_c^* fixed for later reference (this formulation allows us to overcome the problem of non-uniqueness of the solution to optimization problem (5)).

3.2 The Input SM-Based Surrogate Model

The input SM aims at reducing misalignment between the fine and coarse models using an affine variable transformation established based on the available fine model data. The surrogate model $\boldsymbol{R}_s^{(i)}$ is defined as

$$\boldsymbol{R}_s^{(i)}(\boldsymbol{x}) = \boldsymbol{R}_c(\boldsymbol{B}^{(i)} \cdot \boldsymbol{x} + \boldsymbol{c}^{(i)}) \qquad (9)$$

$$(\boldsymbol{B}^{(i)}, \boldsymbol{c}^{(i)}) = \arg\min_{(\boldsymbol{B},\, \boldsymbol{c})} \varepsilon^{(i)}(\boldsymbol{B}, \boldsymbol{c}) \qquad (10)$$

where matrices $\boldsymbol{B}^{(i)} \in \mathbb{R}^{n\times n}$ and $\boldsymbol{c}^{(i)} \in \mathbb{R}$ are obtained using parameter extraction applied to the matching condition $\varepsilon^{(i)}$. Matching condition $\varepsilon^{(i)}$ determines the surrogate model as much as formula (9) does. We can consider different matching conditions that aim to match the fine and surrogate model responses and/or their first-order derivatives. A general form of the matching condition is

$$\varepsilon^{(i)}(\boldsymbol{B}, \boldsymbol{c}) = \sum_{k=0}^{i} w_k \|\boldsymbol{R}_f(\boldsymbol{x}^{(k)}) - \boldsymbol{R}_c(\boldsymbol{B} \cdot \boldsymbol{x}^{(k)} + \boldsymbol{c})\|$$
$$+ \sum_{k=0}^{i} v_k \|\boldsymbol{J}_{\boldsymbol{R}_f}(\boldsymbol{x}^{(k)}) - \boldsymbol{J}_{\boldsymbol{R}_c}(\boldsymbol{B} \cdot \boldsymbol{x}^{(k)} + \boldsymbol{c}) \cdot \boldsymbol{B}\| \qquad (11)$$

We assume that coefficients w_k and v_k are either 0 or 1 (although more general situations are conceivable in practice). Setting $w_k = 1, k = 0, \ldots, i$ and $v_k = 0, k = 0, \ldots, i-1, v_i = 1$ means that the surrogate tries to match the fine model response at all previous points $\boldsymbol{x}^{(k)}$ (including the current point) as well as the Jacobian at the current point.

3.3 The Output SM-Based Surrogate Model

The output space mapping (OSM) aims at reducing misalignment between the coarse and fine models by adding a difference (residual) between those two to $\boldsymbol{R}_c$. We define function $\Delta\boldsymbol{R} : X_f \cap X_c \to \mathbb{R}^m$ as

$$\Delta\boldsymbol{R}(\boldsymbol{x}) = \boldsymbol{R}_f(\boldsymbol{x}) - \boldsymbol{R}_c(\boldsymbol{x}) \qquad (12)$$

We construct surrogates that use (local) models of $\Delta\boldsymbol{R}$, denoted as $\Delta\boldsymbol{R}_m$. A generic surrogate model defined by OSM is

$$\boldsymbol{R}_s^{(i)}(\boldsymbol{x}) = \boldsymbol{R}_c(\boldsymbol{x}) + \Delta\boldsymbol{R}_m(\boldsymbol{x}, \boldsymbol{x}^{(i)}) \qquad (13)$$

We consider the zero-order model $\Delta \boldsymbol{R}_m(\boldsymbol{x}, \boldsymbol{x}^{(i)}) = \Delta \boldsymbol{R}(\boldsymbol{x}^{(i)})$ which leads to the surrogate

$$\boldsymbol{R}_s^{(i)}(\boldsymbol{x}) = \boldsymbol{R}_c(\boldsymbol{x}) + \Delta \boldsymbol{R}(\boldsymbol{x}^{(i)}) \tag{14}$$

The second model is a first-order approximation of $\Delta \boldsymbol{R}$ of the form $\Delta \boldsymbol{R}_m(\boldsymbol{x}, \boldsymbol{x}^{(i)}) = \Delta \boldsymbol{R}(\boldsymbol{x}^{(i)}) + \boldsymbol{J}_{\Delta \boldsymbol{R}}(\boldsymbol{x}^{(i)}) \cdot (\boldsymbol{x} - \boldsymbol{x}^{(i)})$, where $\boldsymbol{J}_{\Delta \boldsymbol{R}}(\boldsymbol{x}^{(i)})$ denotes the Jacobian of $\Delta \boldsymbol{R}$ at $\boldsymbol{x}^{(i)}$. This leads to the surrogate

$$\boldsymbol{R}_s^{(i)}(\boldsymbol{x}) = \boldsymbol{R}_c(\boldsymbol{x}) + \Delta \boldsymbol{R}(\boldsymbol{x}^{(i)}) + \boldsymbol{J}_{\Delta \boldsymbol{R}}(\boldsymbol{x}^{(i)}) \cdot (\boldsymbol{x} - \boldsymbol{x}^{(i)}) \tag{15}$$

Instead of the exact Jacobian (usually unavailable) we can use its approximation produced by the Broyden update.

3.4 The Implicit SM-Based Surrogate Model

Implicit space mapping (ISM) makes use of additional parameters available in the coarse model, i.e., we have $\boldsymbol{R}_c : X_c \times X_p \to \mathbb{R}^m$ where $X_p \subseteq \mathbb{R}^q$ is the domain of such preassigned parameters. Preassigned (non-optimized) parameters abound in engineering design. Their successful exploitation as surrogate modeling parameters depends on much the same engineering expertise required in designating the optimization variables themselves.

An ISM optimization algorithm aims at predistortion of the coarse model by adjustment of certain preassigned parameters $\boldsymbol{x}_p$ so that, at the current point $\boldsymbol{x}^{(i)}$, the fine and coarse model response vectors are aligned. The predistorted model becomes a surrogate which, in turn, is optimized in order to obtain the next point $\boldsymbol{x}^{(i+1)}$. Thus, the surrogate model defined by ISM is

$$\boldsymbol{R}_s^{(i)}(\boldsymbol{x}) = \boldsymbol{R}_c(\boldsymbol{x}, \boldsymbol{x}_p^{(i)}) \tag{16}$$

where $\boldsymbol{x}_p^{(i)}$ is determined by solving a PE problem of the form

$$\boldsymbol{x}_p^{(i)} = \arg \min_{\boldsymbol{x} \in X_p} \|\boldsymbol{R}_f(\boldsymbol{x}^{(i)}) - \boldsymbol{R}_c(\boldsymbol{x}^{(i)}, \boldsymbol{x})\| \tag{17}$$

3.5 SM Surrogate Models Based on Combined Concepts

It is possible and utilized in practice to combine the concepts discussed so far. For example, one can define the ith surrogate $\boldsymbol{R}_s^{(i)}$ using input, output and implicit SM as follows

$$\boldsymbol{R}_s^{(i)}(\boldsymbol{x}) = \boldsymbol{R}_c(\boldsymbol{B}^{(i)} \cdot \boldsymbol{x} + \boldsymbol{c}^{(i)}, \boldsymbol{x}_p^{(i)}) + \boldsymbol{d}^{(i)} + \boldsymbol{E}^{(i)} \cdot (\boldsymbol{x} - \boldsymbol{x}^{(i)}) \tag{18}$$

where matrices $\boldsymbol{B}^{(i)}$ and $\boldsymbol{c}^{(i)}$ as well as preassigned parameter values $\boldsymbol{x}_p^{(i)}$ are determined using parameter extraction (see (10), (11) and (17), respectively), while $\boldsymbol{d}^{(i)} = \boldsymbol{R}_f(\boldsymbol{x}^{(i)}) - \boldsymbol{R}_c(\boldsymbol{B}^{(i)} \cdot \boldsymbol{x}^{(i)} + \boldsymbol{c}^{(i)}, \boldsymbol{x}_p^{(i)})$, $\boldsymbol{E}^{(i)} = \boldsymbol{J}_{\boldsymbol{R}_f}(\boldsymbol{x}^{(i)}) - \boldsymbol{J}_{\boldsymbol{R}_c}(\boldsymbol{B}^{(i)} \cdot \boldsymbol{x}^{(i)} + \boldsymbol{c}^{(i)}, \boldsymbol{x}_p^{(i)}) \cdot \boldsymbol{B}^{(i)}$.

Combining different kinds of space mapping allows us to improve the flexibility of the surrogate model. On the other hand, the proper choice of the SM used to construct the surrogate, as well as the amount of fine model data used in this process, is usually problem dependent and knowledge of the problem and engineering experience are key factors to making this choice successful.

4. Conclusions

We have reviewed the space mapping approach to engineering surrogate modeling and design optimization. As with other surrogate methodologies, the aim is to avoid expensive direct optimization of high-fidelity models. In space mapping, we represent the objective function and constraint functions over a region of the design space through the construction of a suitably accurate physics-based surrogate. Instead of optimizing the high-fidelity model, we optimize the surrogate, which can further be refined as increasingly accurate model data becomes available. The notion of parameter extraction is important to space mapping. Here, high-fidelity data is exploited to validate the design and to improve the local alignment between the surrogate and the high-fidelity model. Using a low-fidelity and physically meaningful model to construct a surrogate is what differentiates space mapping from many other surrogate-based optimization methods. We have reviewed the original formulation as well as the so-called input, output and implicit formulations. Space mapping allows an engineer to exploit his/her detailed knowledge of the engineering design problem.

Matlab engines to implement the current state of the art (several dozen space mapping algorithms and models) to exploit full-wave electromagnetic simulators and fast, empirical, coarse or surrogate device models are under development. This endeavour is designed to make our technology universally available. The reader interested in this software should contact the first author.

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