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Original article

Manifold mapping optimization with or without true gradients

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Abstract

This paper deals with the space mapping optimization algorithms in general and with the manifold mapping technique in particular. The idea of such algorithms is to optimize a model with a minimum number of each objective function evaluations using a less accurate but faster model. In this optimization procedure, fine and coarse models interact at each iteration in order to adjust themselves in order to converge to the real optimum. The manifold mapping technique guarantees mathematically this convergence but requires gradients of both fine and coarse model. Approximated gradients can be used for some cases but are subject to divergence. True gradients can be obtained for many numerical model using adjoint techniques, symbolic or automatic differentiation. In this context, we have tested several manifold mapping variants and compared their convergence in the case of real magnetic device optimization.

Keywords: Space mapping; Surrogate model; Gradients; Symbolic derivation; Automatic differentiation

1. Introduction

The space-mapping technique [1] allows computationally expensive simulation based optimization procedures to be speeded up through the use of approximate models. In the space mapping literature the so-called fine and coarse models are conceived as mappings from the design space to the space of model responses. The key element is the space mapping function. It reparametrises the coarse model domain in such a way to minimize the discrepancy between the fine and coarse model responses. The composition of the space-mapping function and the coarse model response defines a surrogate for the fine model. Instead of solving the fine model problem directly, space-mapping solves the surrogate optimization problem through a sequence of approximations of the space-mapping function. This in turn defines a sequence of coarse model optimization problems whose solution by definition converges to the space-mapping solution. The computational efficiency of this procedure stems from the fact that it takes less fine model evaluations to converge than it takes to solve the fine model optimization problem. The drawback is that the space-mapping solution does not necessarily coincide with the fine model optimum.

In the manifold-mapping technique [6], the surrogate model is constructed in such a way that in a neighbourhood of the fine model optimum, the surrogate model response closely resembles its fine model counterpart. This guarantees that the solutions of the surrogate and fine model optimization problem do coincide. The space-mapping function is replaced

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by the so-called manifold-mapping function. The latter is an affine transformation between the tangent manifolds of the fine and coarse model image spaces. Manifold-mapping is computationally as efficient as space-mapping.

Space mapping techniques have been used in electromagnetic device optimization for several years now [3,7,8,12,14]. Different techniques can be used, but manifold mapping, which is the only one proved to converge to the fine model optimum is always using approximated gradients of the fine model since true gradients are not always available.

This paper details the manifold mapping technique and argues that exact gradients can be available more or less easily nowadays. The computational cost of these gradients is generally small compared with that of the fine model, and the convergence of the manifold mapping algorithm is improved. This property will be required in the future when optimization specifications becomes more and more constrained.

2. Manifold mapping algorithm

2.1. Mathematical background

Let us consider an optimization problem with design variables x in the design space $x \in X \subset \Re^n$ and specifications $y \in \Re^m$ which can be approximated by minimizing a cost functional $F(x) \in \Re$ (e.g. Eq. (4)).

The manifold-mapping function $S : c(X) \mapsto f(X)$ is a mapping between the coarse model $c(X) \subset \Re^m$ and fine model $f(X) \subset \Re^m$ image spaces. This function maps the point $c(x_f^*)$ to $f(x_f^*)$ and the coarse model tangent space at $c(x_f^*)$ to the fine model tangent space at $f(x_f^*)$. It allows to define the surrogate model $S(c(x))$ and to write the manifold-mapping solution as follows:

$$\begin{aligned} &\text{find } x_{mm}^* \in X \quad \text{such that} \\ &x_{mm}^* = arg \min_{z \in X} ||S(c(z)) - y|| \end{aligned} \tag{1}$$

The manifold-mapping function $S(x)$ is approximated by a sequence $\{S_k(x)\}_{k\geq 1}$ yielding a sequence of iterands $\left\{x_{k,mm}\right\}_{k\geq 1}$ converging to x_{mm}^*. The individual iterands are defined by coarse model optimization:

$$\begin{aligned} &\text{find } x_{k,mm}^* \in X \quad \text{such that} \\ &x_{k,mm}^* = arg \min_{z \in X} ||S_k(c(z)) - y|| \end{aligned} \tag{2}$$

At each iteration k, the construction of S_k is based on tangent planes of coarse and fine model, i.e., $S_k = J_c(x_k^*) \cdot J_f^+(x_k^*)$ where the matrices $J_c(x_k^*)$ and $J_f^+(x_k^*)$ of size $m \times n$ are the Jacobian of $c(x_k)$, and pseudo inverse of the Jacobian of $f(x_k)$, respectively. The pseudo inverse can be computed by a simple QR decomposition or using the singular value decomposition.

If the Jacobians are not available, S_k can be approximated using ΔC and ΔF of size $m \times \min(k, n)$ defined as follows:

$$\Delta C = [c(x_k) - c(x_{k-1}), c(x_k) - c(x_{k-2}), \ldots, c(x_k) - c(x_{\max(k-n,0)})]$$

$$\Delta F = [f(x_k) - f(x_{k-1}), f(x_k) - f(x_{k-2}), \ldots, f(x_k) - f(x_{\max(k-n,0)})]$$

During the first n iterations, these matrices are not fully describing the tangent planes but are enough to define a search direction until k becomes greater than n.

In order to improve robustness of the approximation S_k is defined with a complementary term $S_k = \Delta C(x_k^*) \cdot \Delta F^+(x_k^*) + (I - U_{k,c}U_{k,c}^T)$ where $U_{k,c}$ is provided by the singular value decomposition of $\Delta C = U_c \cdot \Sigma_c \cdot V_c^T$ at each k iteration.

Using S_k mapping function, an update objective $y_k = c(x_k) - S_k(f(x_k) - y)$ can be introduced leading to an asymptotically equivalent problem:

$$\begin{aligned} &\text{find } x_{k,mm}^* \in X \quad \text{such that} \\ &x_{k,mm}^* = \arg \min_{z \in X} ||c(z) - y_k|| \end{aligned} \tag{3}$$