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ANOVA EXPANSIONS AND EFFICIENT SAMPLING METHODS FOR PARAMETER DEPENDENT NONLINEAR PDES

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Abstract. The impact of parameter dependent boundary conditions on solutions of a class of nonlinear partial differential equations and on optimization problems constrained by such equations is considered. The tools used to gain insights about these issues are the Analysis of Variance (ANOVA) expansion of functions and the related notion of the effective dimension of a function; both concepts are reviewed. The effective dimension is then used to study the accuracy of truncated ANOVA expansions. Then, based on the ANOVA expansions of functionals of the solutions, the effects of different parameter sampling methods on the accuracy of surrogate optimization approaches to constrained optimization problems are considered. Demonstrations are given to show that whenever truncated ANOVA expansions of functionals provide accurate approximations, optimizers found through a simple surrogate optimization strategy are also relatively accurate. Although the results are presented and discussed in the context of surrogate optimization problems, most also apply to other settings such as stochastic ensemble methods and reduced-order modeling for nonlinear partial differential equations.

Key Words. ANOVA expansions, nonlinear partial differential equations, surrogate optimization, parameter sampling methods.

1. Introduction

The type of problems we consider requires the solutions of equations such as

$$F(u; \vec{\alpha}) = 0, \tag{1}$$

where $\vec{\alpha} \in A \subseteq \mathbb{R}^p$ is a vector of parameters and A is some admissibility set. In particular, we are interested in problems for which $F(\cdot; \vec{\alpha})$ represents a nonlinear partial differential equation or system. The specific situation that interests us is one in which approximate solutions of problems involving (1) are determined by using the solutions to the problems

$$F(u^{(j)}; \vec{\alpha}^{(j)}) = 0 \quad j = 1, \dots, N, \tag{2}$$

where $\{\vec{\alpha}^{(j)}\}_{j=1}^{N}$ are a chosen set of parameter values. Settings in which such problems arise include ensemble approximations of solutions of (1) in case the components of the parameter vector $\vec{\alpha}$ are random variables with given probability distributions; building reduced-order models from solutions of (1) at sample values

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of the parameter vector $\vec{\alpha}$; and the surrogate optimization of a functional. Here, we focus on the third setting; however, most of the discussions in this paper can be translated to the other settings.

For surrogate optimization problems, we are given a functional $\mathcal{J}(u)$ and are asked to find $\vec{\alpha}^* \in A$ and a corresponding u^* that solve the problem

$$\min_{\vec{\alpha}\in A} \mathcal{J}(u) \quad \text{subject to} \quad F(u;\vec{\alpha}) = 0, \tag{3}$$

where A is a bounded subset of $\mathbb{R}^p$. In this setting, u denotes the state variable, $\vec{\alpha}$ the vector of design parameters, and the constraint equation $F(u;\vec{\alpha}) = 0$ the state system. Note that through the constraint, the functional $\mathcal{J}(u)$ is implicitly a function of the components of the parameter vector $\vec{\alpha}$. A simple, derivative-free approach to finding approximate solutions of the problem (3) is to *first choose particular values* $\{\vec{\alpha}^{(j)}\}_{j=1}^N$ *for the parameters*, then solve the problems in (2), and then use those solutions to evaluate the functional so that one obtains, for $j = 1,\dots,N$, the values $\mathcal{J}(u^{(j)})$ corresponding to the parameter vectors $\vec{\alpha}^{(j)}$. One would then use this information to build, e.g., by a least-squares or interpolatory method, a surrogate function $\mathcal{J}_{sur}(\vec{\alpha})$ defined over the parameter subset A that can be used as an approximation to $\mathcal{J}(u(\vec{\alpha}))$ over A. Finally, one would approximate the solution of the optimization problem (3) by the parameter values that minimize the simpler functional $\mathcal{J}_{sur}(\vec{\alpha})$, i.e.

$$\vec{\alpha}^* \approx \vec{\alpha}^*_{sur}, \quad \text{where } \vec{\alpha}^*_{sur} \text{ solves the problem} \quad \min_{\vec{\alpha}\in A} \mathcal{J}_{sur}(\vec{\alpha}). \tag{4}$$

Building the surrogate functional requires the evaluation of the functional $\mathcal{J}(\cdot)$ at the points $\{\vec{\alpha}^{(j)}\}_{j=1}^N$ sampled within the set A. In turn, evaluating the functional at the N parameter points requires N solves of the constraint equation as in (2). Since the latter step involves solving a nonlinear partial differential equation system, it dominates the overall computation; thus, the constraint equation should be solved as few times as possible. Thus, we want to sample only a "few" points in A, i.e., we want to sample sparsely. In addition, in practice, p, the number of control parameters, may be large so that, for the surrogate optimization problem, we are interested in intelligent, *sparse sampling in possibly high dimensions.*

In this paper, we treat a simple model problem, but the need for intelligent sampling would be even greater in more complicated settings. We even simplify things some more by assuming that the parameter vector is constrained to belong to a hypercube, that its components have no known bias or correlation so that we will sample them uniformly and independently, and that they appear linearly in the definition of the problem. Clearly, this work is only the beginning of what should be a much larger study that encompasses more general and more realistic situations.

The particular focus of this paper is to explore the connections that ANOVA (Analysis of Variance) expansions of multivariate functions (and the related notion of the effective dimension of those functions) have with the solution of parameter-dependent nonlinear partial differential equations. Specifically, we will study the general approximation properties of ANOVA expansions for functionals of solutions of nonlinear partial differential equations and the implications that particular features these expansions possess have on those solutions and on how one builds surrogate functionals.

Of course, the problem of solving partial differential equations with parameter-dependent input data is an active research area; see e.g., [1, 4, 12–15, 17, 19–22, 26, 28, 29]. However, these works are mostly focused at finding approximate solutions