Active Subspace Identification in Surrogate Modeling

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***Abstract*— Many applications and analysis techniques in science and engineering use simulation as a means for gauging a system's behavior. In coarse designs, simulation provides a qualitative look at system attributes. Much denser simulation might be required for more quantitative assessments. However, in advanced simulation techniques with complex models, each simulation can take hours or days. Processes with many variables require many simulation runs to adequately cover the space of responses. In this case, even if each simulation only takes a few minutes, the total simulation time can grow exponentially.**

Surrogate modeling is the technique of creating an algebraic approximation to the simulation's map from parameters to response. The resulting *response surface* or *surrogate model* is much more efficient to evaluate than the original simulation and can provide much insight into the behavior of the original system [7]. The best form for a surrogate model depends on the application. They are formed with various methods such as standard regression, support vector machines [12], and kriging methods [8]. Data Collaboration techniques [3] use quadratic and rational-quadratic surrogate models to calculate outer bounds to various optimization objectives such as the consistency measures and response prediction.

One of the major problems facing surrogate modeling occurs when long simulation time is required to adequately sample the model response. To fit a surrogate model, many simulation runs are often required. The number of simulations can depend on the form of the surrogate (e.g., the number of basis functions) and the dimension of the parameter vector. For example, with a quadratic surrogate, the number of basis functions (monomials with a degree of at most 2) increases quadratically with the number of parameters.

This talk describes a technique for discovering the possible dependence of the response to a lower-dimensional active subspace of the parameters. If such an active subspace were known, the amount of simulation required to make a surrogate would depend on the subspace dimension rather than the original full dimension. The procedure determines if the gradient of the function is confined to a subspace, from which the active subspace can be identified.

Subspace dependence is not a new concept. However, the focus of many studies is on searching for a subspace dependence of the multivariate output of a function or of the evolving state vector of a set of coupled ODEs [1], [5], [6]. Some works use local subspace dependence to preserve neighborhood relationships and fit low-dimensional nonlinear manifolds to the data [2], [4], [11]. High-dimensional model representations (HDMRs, [9], [10]) build up a surrogate model by iteratively fitting along every coordinate-aligned subspace starting with the 0-dimensional subspace.

The talk will outline the procedure and derivation, and a simple complexity analysis. We illustrate the method's behavior on a wide variety of problems, including hydrogen and methane combustion models.

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