Active Subspaces

Emerging Ideas for Dimension Reduction in Functions of Several Variables

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Abstract

The goal of uncertainty quantification (UQ) is to formulate confidence metrics for computer simulations comparable to those for experiments. In practice, computing these UQ metrics involves parameter studies—e.g., numerical integration, numerical optimization, calibration, or response surface construction. But performing these parameter studies becomes increasingly difficult as the number of input parameters increases, especially when the simulation is expensive. The benefits of dimension reduction cannot be overstated. If one is able to approximate a 10-parameter simulation's prediction by a comparable interface with 2 parameters, then several otherwise intractable techniques become feasible.

I will treat this problem like *approximation*. In particular, I denote the simulation's scalar-valued output that depends on m inputs as a function $f(\mathbf{x})$. I approximate f as

$$f(\mathbf{x}) \;\approx\; g\left(\mathbf{W}^T\mathbf{x}\right), \tag{1}$$

where g is a function of $n < m$ variables, and $\mathbf{W}$ contains the first n eigenvectors of the symmetric, positive semidefinite matrix

$$\mathbf{C} \;=\; \int \nabla f(\mathbf{x})\, \nabla f(\mathbf{x})^T\, \rho(\mathbf{x})\, d\mathbf{x}. \tag{2}$$

The weight function ρ is chosen such that $\mathbf{C}$ is the average of the outer product of gradient with itself. The *active subspace* is defined as the span of the columns of $\mathbf{W}$.

I will discuss our research efforts and progress on active subspaces for dimension reduction with an emphasis on numerical methods. The idea is to discover and exploit important linear combinations of the input parameters to reduce the effort for thorough parameter studies in complex simulations.