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Active Subspace Embedding for Parsimonious Gaussian Process Surrogates

Uncertainty quantification for complex physical systems often relies on computationally expensive numerical simulators. When execution times limit the number of feasible runs, **surrogate modeling** becomes essential for tasks such as sensitivity analysis, design optimization, and safety assessment. **Gaussian process regression (GPR) is a leading surrogate** due to its uncertainty quantification capabilities and flexibility. However, high input dimensionality—common in industrial applications—poses significant challenges: increased computational cost, deteriorated prediction accuracy, and numerical instability in covariance estimation.

We propose a dimension reduction methodology combining **statistical screening and active subspace (AS) identification to enable efficient and parsimonious GPR metamodeling in large-dimensional contexts**. The approach proceeds in three stages: (1) initial variable screening via independence tests based on Hilbert-Schmidt Independence Criterion (HSIC) reduces dimensionality to a tractable scale (~20 variables), (2) a medium-dimensional GPR is fitted to estimate gradient information, from which the gradient covariance matrix and its active subspace decomposition are computed, and (3) a final parsimonious low-dimensional GPR is constructed on the identified active directions. Key methodological contributions include optimal dimension selection via cross-validation adapted to the given-data context, and covariance modeling recommendations tailored to each stage: high-regularity kernels for stable gradient estimation, and flexible kernel choices for final surrogate construction.

We illustrate the methodology on a **nuclear safety application**: peak cladding temperature prediction during intermediate-break loss-of-coolant accidents (IB-LOCA) using the a thermal-hydraulic code. Starting from several dozens of uncertain input parameters, our approach achieves a four-fold dimension reduction yielding a parsimonious surrogate while preserving accuracy and reliable predictive intervals.

Special/ Invited session

Invited session FrEnbis

Classification

Both methodology and application

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