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Spectral Clustering for Detecting Stationary Subregions in Gaussian Process Regression

Complex physical systems are often modeled using high-fidelity simulation codes. However, their inherent complexity makes each simulation computationally expensive, which severely limits their direct use in tasks such as uncertainty quantification. To overcome this, a widely adopted solution is to approximate the simulator using a Gaussian Process Regression (GPR) surrogate model.

However, when the underlying simulation exhibits heterogeneous behaviour over the input domain, such as in two-phase fluid mechanics where flow regime may vary, a standard GPR model with a stationary covariance function may struggle to accurately represent it. In such cases, more sophisticated non-stationary GPR models should be considered. Several approaches have been proposed in the literature, some of which rely on firstly identifying stationary subregions through clustering methods applied to input–output pairs.

These methods typically group points based solely on proximity in the joint input–output space, without explicitly incorporating information about what characterises a shared stationary regime.

To address this limitation, we propose to perform the clustering step using local features as variances and gradients rather than raw outputs, thereby making the clustering process more consistent with the notion of stationarity. In addition, we propose the use of a spectral clustering approach to better account for variations in cluster density induced by local features, while promoting spatial contiguity within the input domain.

The proposed methodology demonstrates encouraging results in moderate dimension for identifying stationary subregions compared to standard approaches, despite the increase in computational complexity.

Special/ Invited session

Classification

Mainly methodology

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