Warwick Centre for Predictive Modelling Seminar Series

Efficient emulation of high-dimensional outputs using manifold learning: Theory and applications

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Abstract: Emulators, also known as surrogate models and metamodels, are approximations of computer models (simulators) and are designed for rapid simulation in applications such as uncertainty analysis, design optimisation and inverse parameter estimation, all of which require simulations at numerous points in a parameter space. Approaches to emulator construction can be classed as either black-box (e.g., polynomial response surface models, support vector machines, Bayesian Gaussian process modelling) or physics-based (typified by reduced basis approximations). When the simulator outputs of interest are one or more spatio-temporal fields (e.g., velocity, pressure, temperature), arising from a system of parameterized partial differential equations (PDEs), enormous challenges are posed in terms of computational efficiency and accuracy. For even moderately coarse spatial discretizations, the dimension of the output space (field variable values at points in a numerical grid) is very large. In problems involving complex geometries or multiple spatial scales, a fine grid may be required to adequately resolve small-scale characteristics. For such problems standard multi-output Gaussian process (GP) emulation strategies are computationally impractical and/or make restrictive assumptions regarding the correlation structure. Methods that rely on a multivariate GP prior with the assumption of a separable covariance structure (the coordinates of the outputs are i.i.d. univariate GPs) for tractability are not suited to highly nonlinear variations in spatial fields. Linear dimensionality reduction of the output space based on principal component analysis avoids this limitation but will fail when the response surface is not faithfully represented by a linear subspace of the ambient space. This could happen if abrupt or highly nonlinear changes take place with variations in one or more input parameters, e.g., transition from subsonic to supersonic flow. In this talk, we describe approaches to Gaussian process emulator construction based on manifold learning methods (nonlinear dimensionality reduction), including kernel PCA, ISOMAP and diffusion maps. The rationale and benefits of the approach are described and its success (computational efficiency and accuracy) in handling complex problems is demonstrated. A strategy to extend the approach to multiple fields using the linear model of coregionalisation is presented. We also discuss our latest efforts to apply manifold learning to physics-based emulation strategies for time-dependent, parameterized PDE problems.

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