Emulation of multivariate simulators using thin plate splines with application to atmospheric dispersion

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It is often desirable to build a statistical emulator of a complex computer simulator in order to perform analysis which would otherwise be computationally infeasible. We propose methodology to model multivariate output from a computer simulator taking into account spatial structure in the responses. The utility of this approach is demonstrated by applying it to a chemical and biological hazard prediction model. Predicting the hazard area which results from an accidental or deliberate chemical or biological release is imperative in civil and military planning and also in emergency response. The hazard area resulting from such a release is highly structured in space and we therefore propose the use of a thin-plate spline to capture the spatial structure and fit a Gaussian process emulator to the coefficients of the resultant basis functions. We compare and contrast three different techniques for emulating multivariate output: a fully Bayesian approach with a principal component basis, a fully Bayesian approach with a thin-plate spline basis, assuming that the basis coefficients are independent and a "plug-in" Bayesian approach with a thin-plate spline basis and a separable covariance structure. We develop methodology for these latter two emulators and demonstrate that a thin-plate spline emulator significantly outperforms the principal component emulator. Further, the separable emulator, which accounts for the dependence between basis coefficients, provides substantially more realistic quantification of uncertainty, and is also computationally more tractable, allowing fast emulation.

Keywords: Computer experiment; dimension reduction; Gaussian process; principal components.