

Computer Emulation with Non-Stationary Gaussian Processes

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Gaussian process (GP) models are widely used to emulate propagation of uncertainty in computer experiments. GP emulation sits comfortably within an analytically tractable Bayesian framework. Apart from propagating uncertainty of the input variables, a GP emulator trained on finitely many runs of the experiment also offers error bars for response surface estimates at unseen input values. This helps select future input values where the experiment should be run to minimize uncertainty in the response surface estimation. However, traditional GP emulators use stationary covariance functions, which perform poorly and lead to sub-optimal selection of future input points when the response surface has sharp local features, such as a jump discontinuity or an isolated tall peak. We propose an easily implemented non-stationary GP emulator, based on two stationary GPs, one nested inside the other, and demonstrate its superior ability in handling local features and selecting future input points from boundaries of such features.

Joint work with Silvia Montagna.