Modelling and sensitivity analysis in computer experiments with quantitative and qualitative inputs

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Abstract

In engineering and natural sciences it has become common practice to replace physical experiments by computer simulations (black-box experiments). As these simulations can be very time-consuming and complex often a surrogate or meta-model of the computer experiment is build first and analysis and optimization are then based on this model. Gaussian process models, better known as Kriging models, are widely used for this purpose. Based on kernels they can be tuned to many situations. The prediction function interpolates the observed data points, which reflects the usually deterministic character of a computer experiment. We present a novel extension of the Kriging model to both quantitative and qualitative inputs based on the Gower distance metric.

Sensitivity analysis is a technique often applied to computer experiments - it explores the effect of controllable parameters on the response variable of interest. We review the Sobol sensitivity indices and the more recently developed total interaction indices (TII) and show different ways to display the result in so called FANOVA graphs. Besides increasing the knowledge about the unknown black-box function the results of the sensitivity analysis can be used within modelling and optimization. We demonstrate how Gaussian process models with a kernel reflecting the additivity structure implicated by the FANOVA graph can improve the goodness of fit