Exploring the limits of metamodels for sensitivity analysis at low sample sizes

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Metamodels are an essential tool for performing sensitivity analysis on models with a large run time, where only a limited number of model runs are available. Of these, Gaussian processes and Polynomial Chaos Expansions are arguably the most prominent approaches. However, even metamodels require a minimum number of model runs to give reliable results: below a certain limit, metamodels can give very inaccurate results, particularly in higher dimensions. At these sample sizes, more accurate results can actually be obtained by simple sample-based approaches.

This lower limit sample size is a function of (at least) the form of the model, and the number of model inputs. Currently, there is no evidence which gives practitioners an idea of where these limits lie, but this is important to know a priori because it dictates the sampling strategy. This work proposes an empirical approach to explore the limits between metamodels and sampling approaches, by running a very large number of sensitivity analyses on problems of varying dimensionality and sample size. A particular novelty here is that a "meta-function" (a function-generating function) is proposed which, to some extent, relaxes the dependence of the results on the test function used. The results allow maps to be drawn which show the boundary lines (in terms of sample size and dimensionality) between where it might be more useful to use a metamodel, and where it is likely better to use simple sampling approaches.