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# Sensitivity analysis of simulation models: an overview

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**Abstract**

This Invited Lecture covers classic and modern designs, and their metamodels. Classic resolution-III designs including fractional-factorial two-level designs assume first-order polynomial metamodels. Resolution-IV and resolution-V designs assume such polynomials augmented with two-factor interactions. Central Composite Designs (CCDs) assume second-degree polynomials. Simulations with many factors require modern factor-screening designs; e.g., sequential bifurcation and Morris's designs. Globally fitted Kriging metamodels require space-filling designs; e.g., Latin Hypercube Sampling (LHS). Sensitivity analysis also serves optimization of the simulated system. Classic Response Surface Methodology (RSM) is popular. Novel methods select one of the multiple simulation outputs as goal variable, and satisfy given constraints on the other outputs and the inputs. Taguchian robust optimization allows for uncertainties in some (environmental) inputs.

*Keywords:* Simulation, sensitivity analysis; gradients; design of experiments; screening; Kriging; optimization; RSM; Taguchi

## 1. Overview

This Invited Lecture gives an overview of *Sensitivity Analysis* (SA) of simulation models (also called computer codes), treating the simulation model as a *black box*; i.e., the SA uses only the Input/Output (I/O) data of the simulation model (not the internal variables and functions). To obtain these I/O data, the SA should use proper *Design Of Experiments* (DOE). This DOE should depend on the (tentative) *metamodel (*also called emulator, response surface, surrogate), which approximates the I/O function that is defined by the underlying simulation model. A *local* experiment may be used to estimate the *gradient*, so the analysts may assume a *first-order polynomial* metamodel. For such a polynomial, a *Resolution-III* (R-III) design suffices; such a design may be a *factorial two-level design*, which consists of all $2^k$ combinations of the two extreme values for each of the $k \geq 1$ "factors" or simulation inputs. Such a design gives more accurate *Ordinary Least Squares* (OLS) estimators of the $k$ first-order or main effects (say) $\beta_j$ ($j$ =1, …, $k$) and the intercept (say) $\beta_0$ than changing one factor at a time; see Kleijnen (2008, p. 29). However, if there are more than two factors ($k > 2$), then only a *fraction* of these $2^k$ combinations needs to be simulated; e.g., if $k = 3$ then there are only 4 effects to be estimated so instead of $2^3$ combinations only $2^{3-1}$ combinations are simulated. In general, some R-III designs or *Plackett-Burman designs* are $2^{k-p}$ *designs* with a proper selection of $p$. However, for $k$ = 11 only 12 instead of $2^{11}$ = 2,048 combinations are needed; obviously, these 12 combinations are not a $2^{k-p}$ design. Both types of R-III designs are tabulated in Kleijnen (2008, pp. 36-40). A first-order polynomial metamodel may turn out not to be *valid*; e.g., the popular coefficient of determination $R^2$ may be much smaller than one, or cross-validation


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gives significant prediction errors; see Kleijnen (2008, pp. 54-63). The analysts may then augment the first-order polynomial with *two-factor interactions* (cross-products). A *Resolution-IV* (R-IV) design then gives OLS estimators of the first-order effects (and the gradient) that are not biased by these two-factor interactions. The computational extra cost is the doubling of the number of combinations (say) $n$: so-called *foldover principle*, which augments the R-III design (say) $\boldsymbol{D}$ with its negative or "mirror image", $-\boldsymbol{D}$; see Kleijnen (2008, pp. 42-43). If the analysts wish to estimate the *individual* two-factor interactions, then they should use *Resolution-V* (R-V) designs, which require the simulation of many more factor combinations because the number of polynomial coefficients or regression parameters (say) $q$ increases to $1 + k + k(k - 1)/2$. Examples are $2^{5-1}$ and $2^{11-4}$ designs; see the table for $5 \leq k \leq 11$ in Kleijnen (2008, p. 48). However, there designs are not so "efficient": $n >> q$. There are also (less popular) *saturated* R-V designs; i.e., design with $n = q$; see Kleijnen (2008, pp. 48-49). The preceding designs of various resolution may be used to find out whether specific factors are *unimportant*; i.e., they have no first-order effects and do not interact with other factors. Some authors call this use of the preceding classic designs *screening*. However, if the number of factors is (say) 1000, then these designs require too much simulation time because they require at least $k + 1$ combinations. The analysts may then use special screening designs; e.g. *sequential bifurcation* and *Morris's design*s; see Kleijnen (2008, pp. 159-172). For the important factors the analysts may assume a *second-order polynomial* metamodel, especially when they wish to estimate the optimal factor values. Unbiased estimators of the polynomial coefficients are provided by the popular *Central Composite Designs* (CCDs). A CCD augments the R-V design with the "central point" $x = 0$ and $2k$ "axial points", which change factor $j$ ($j = 1, \ldots, k$) from its central value 0 to $-c$ and $c$ respectively with $c \neq 0$, while keeping the other $k - 1$ factors at their central values. Note that all factor values in the various designs are *standardized* between (say) -1 and 1; see Kleijnen (2008, pp. 29-32). All these classic designs assume low-order polynomials plus *white noise* so OLS gives optimal estimators; otherwise the analysts may apply either Weighted or Generalized Least Squares, bootstrapping, etc.; see Kleijnen (2008, pp. 73-100).

Besides first-order or second-order polynomial metamodels, there are many *modern* types of metamodels; see Kleijnen (2008, p. 8). The most popular alternative is the *Kriging* (or Gaussian Process) metamodel (named after Danie Krige). Such a metamodel gives a good global fit over a large experimental area. Mathematically, Kriging uses a linear combination of the $n$ "old" simulation outputs, to predict the output for the "new" input combinations where the weights decrease as the old input combination lies farther away from the new input combination. The optimal weights are estimated assuming a specific *covariance stationary process* that quantifies how the correlations among outputs vary with the distance among their inputs. To compute the Kriging metamodel, the analysts can use free and well-documented Matlab Kriging software called *DACE*. Designs for generating the necessary I/O simulation data (to be analyzed by Kriging) are *space filling*. The most popular design is *Latin Hypercube Sampling* (LHS), for which there is ample software. However, *sequential designs* are more efficient, because they analyze the available I/O data before selecting the next input combination. Details on Kriging metamodels and their designs are given by Kleijnen (2008, pp. 139-156).

SA may also serve *optimization* of the simulated system. A classic method is *Response Surface Methodology* (RSM), which is a stepwise heuristic that starts with a local experiment using a R-III design, estimates the gradient, changes the factors through Steepest Ascent, and ends with a second-order polynomial to estimate the optimum. Modern variants allow for *multiple* simulation outputs, and select one output as the goal while satisfying constraints on the remaining outputs and on the $k$ inputs. These variants either generalize RSM or fit a Kriging metamodel for each of the multiple simulation outputs, and combines these Kriging models with a Nonlinear Programming algorithm to estimate the optimum. Finally, *robust* optimization also accounts for *uncertainty* in the environmental inputs, which are beyond management's control. Optimization is discussed by Kleijnen (2008, pp. 101-138).

## 2. References

Kleijnen, J.P.C., 2008, *Design and analysis of simulation experiments*, Springer