An efficient methodology for modeling complex computer codes with gaussian processes

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Abstract

Many physical phenomena are investigated by deterministic equations which lead to the implementation of computer codes. These computer codes are often complex, time expensive and consequently not directly usable to conduct studies like uncertainty propagation or global sensitivity analysis. So, it can be useful to replace this complex code by an approximated model called response surface. This function must be representative of the computer code and require a negligible calculation time.

Since the computer codes considered here are supposed deterministic, it would be interesting to use an exact interpolator as response surface. Moreover, as our study comes within the scope of sensitivity analysis and uncertainty propagation, it is very useful to dispose of an analytic predictor formula. For all these reasons, the gaussian process model, which is an extension of kriging to computer codes, appears as an interesting candidate.

Indeed, numerous authors like Currin et al.[1], Santner et al.[2] and Vazquez et al.[3] show how this model can provide a statistical basis for computing an efficient predictor of code response. In a recent study concerning the modeling of pollutant migration in soils, I developp a methodology to substitute gaussian process model to a classical hydrogeologic software. All the modeling procedure will be described, from the model estimation to its validation passing through the input variable selection. Then, the exploitation of this gaussian process model to make a sensitivity analysis or an uncertainty propagation will be introduced.

Keywords: gaussian process, kriging, response surface, computer codes, uncertainty, sensitivity analysis, covariance, variable selection.

References

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