

Surrogate models, or metamodels, are compact analytical models that approximate the multivariate input/output behavior of complex systems based on a limited set of computationally expensive simulations. The idea of the surrogate is that it mimics the complex behavior of the underlying simulation model, but it is computationally inexpensive by comparison. It is useful for parametric studies, trade space exploration, and sensitivity analysis as it can be exercised rapidly and, in general, has second-order continuous derivatives.

The concern with surrogate modeling is that it is being used indiscriminately. It is oft heard that a researcher “sequentially built a meta-model to optimize the objective functions”, but there is little said of whether this was necessary or efficient. In fact, all surrogate modeling techniques are interpolating schemas so to optimize one is trivial. What is optimized is the uncertainty, or maximum-likelihood estimator as in (Super)EGO, to match the metamodel representation of the objective space to the true topology. Optimizing the metamodel alone places too much emphasis on exploiting the predictor rather than exploring regions of the space that are uncertain.

This paper discusses the computational cost of developing metamodels. Radial basis functions are used as example kernels for estimating the cost of: (1) surrogate regression; (2) surrogate evaluation; (3) maximum likelihood estimator for improvement; and (4) accrued cost of sequentially building the regression. It is shown that the surrogate-regression is linear in the dimension of the input space and of order 3 with respect to the number of training points.