Rational function approximations in a response surface methodology

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Abstract: Scenario analyses of complex dynamic systems, such as environmental and economic systems, can be very computationally demanding and can generate large amounts of data. To efficiently process and summarize the results from such a scenario analysis, a response surface methodology (RSM) has been proposed. The RSM has originally been used to support efficient experimentation, but extensions towards efficient numerical experimentation have been widely accepted (Kleijnen, JPC (2008) Design and Analysis of Simulation Experiments, Springer Verlag, pp. 216). After sampling the factor space and subsequently conducting the (numerical) experiments, the resulting responses form the so-called response surface that is typically approximated by a multivariate polynomial function.

Polynomial models are frequently used for curve fitting, as these models have a simple form, have well-known properties, have moderate flexibility of shapes, are a closed family and computationally easy to use. However, polynomial models have poor interpolatory and extrapolatory properties, have poor asymptotic properties and exhibit a poor trade-off between shape and degree. Nevertheless, second-order polynomial models are popular, as these allow nice interpretations, even for high-dimensional factor spaces. For instance, an eigenvalue decomposition of the matrix weighting the second-order terms provides the orientation of the main axes and corresponding lengths of the semi-axes of the approximate ellipsoidal surfaces.

Rational functions for approximate modelling of a response surface will, in general, give better fits than polynomial functions. A rational function is simply the ratio of two polynomial functions. Rational function models have a moderately simple form, are a closed family, can take on an extremely wide range of shapes, have better interpolatory and extrapolatory properties than polynomial models and have excellent asymptotic properties. As for the polynomial model, the coefficients of a rational model and their statistical properties can, after a linear parametrization, be estimated using ordinary least-squares methods. Refer to Doeswijk, TG, Keesman, KJ (2009) Linear parameter estimation of rational biokinetic functions. Water Research 43 (1), 107 – 116) for further details.

The objective of this work was to introduce rational function approximations in RSM and, in particular, to present some properties of a rational function composed of two second-order polynomials. A truncated two-dimensional Gaussian function (Figure 1), typically found in solving diffusion problems, will be presented to demonstrate the advantage of using a rational instead of a polynomial approximation.

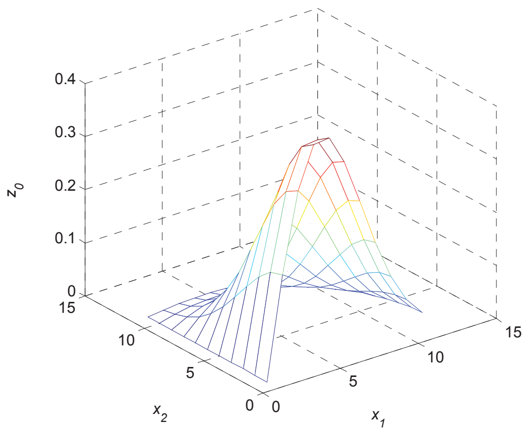

Figure 1. Example response surface.

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