Taylor Kriging Metamodelling for Stochastic Simulation Interpolation

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ABSTRACT

This paper applies a novel Kriging model to the interpolation of stochastic simulation with high computational expense. The novel Kriging model is developed by using Taylor expansion to construct a drift function for Kriging, thus named Taylor Kriging. The interpolation capability of Taylor Kriging for stochastic simulation is empirically compared with those of Simple Kriging and Ordinary Kriging according to two stochastic simulation cases. Results show that the interpolation of Taylor Kriging is more accurate than Simple Kriging and Ordinary Kriging. The authors analyze two key factors in stochastic simulation, simulation replications and variance, which influence the accuracy of Kriging interpolation, and obtain some important empirical results.

Keywords: Accuracy, Interpolation, Simulation Replications, Stochastic Simulation, Taylor Kriging

INTRODUCTION

Simulation models can consider the details and constraints of simulated systems and thus are able to effectively describe simulated systems. Due to the complexity of simulated systems, corresponding simulation models are often computationally expensive and interpolation thus becomes critical. Recently, Kriging has been applied to simulation interpolation because of its accurate nonlinear interpolation capability. Kriging is named after Krige, a mining engineer in South Africa (Krige, 1951).

The application of Kriging in simulation interpolation initially occurred in the deterministic area. The representative work is given by Sacks, Welch, Mitchell, and Wynn (1989) who consider experiments which are computationally expensive to run and whose outputs are deterministic. For such computer experiments, Sacks et al. (1989) use Kriging to fit an inexpensive but efficient predictor to reduce their computational cost. Mitchell and Morris (1992) investigate Kriging as an alternative to conventional response surface methodology for use in simulation experiments. Mitchell and Morris treat Kriging as a Bayesian method. They use Kriging to evaluate the importance of input parameters, consider how to use Kriging to optimize a dependent variable in the interested

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region of independent variables in the space of input parameters, and discuss the application of Kriging in inverse problems according to a simulation experiment on the model of groundwater flow. Their work focuses on deterministic simulation interpolation. However, they indicate that some modifications can be made so that Kriging can handle the simulation interpolation with stochastic outputs. Trochu, Sacepe, Volkov, and Turenne (1999) use Dual Kriging as an interpolation method to simulate the macroscopic mechanic behavior of shape memory alloys. They apply Dual Kriging to yielding the explicit equation of any partial cycle inside the main hysteretic domain, thus presenting a general material law for shape memory alloys.

The early application of Kriging to stochastic simulations was proposed by Barton (1994). In his introduction to Kriging, he regards Kriging as a spatial correlation metamodel. Barton indicates that although the fitting capability of the spatial correlation method is exciting, it is based on a small set of examples, and the more extensive computational comparison of the methods would have to wait for more generally available computer codes. Régnire and Sharov apply Kriging to interpolating the spatial and temporal output data of the simulation model for male gypsy moth flight phenology (1999). Universal Kriging (UK) and multivariate linear regression are compared in their simulation interpolation. Based on experimental results, they think that these two methods are nearly equally precise in interpolating the output data of a simulation model; Kriging models require more computing time than does regression. They believe that the success of regression may be due to the relatively simple physical processes simulated, and UK offers an alternative in cases where simple polynomial terms cannot mimic more complex response surfaces. As van Beers and Kleijnen (2004) later indicated, the multivariate linear regression compared with UK by Régnire and Sharov is a rather complicated metamodel (involving terms of order six), which is perhaps one reason why its resulting interpolation accuracy is similar to that of Kriging.

Meckesheimer and Booker (2002) develop efficient methods to assess the validity of Kriging and other metamodels in simulation interpolation. They investigate computationally inexpensive assessment methods for metamodel validation based on leave-k-out cross validation, and develop guidelines about how to select k. Based on the results from two sets of test problems, \( k = 0.1N \) or the square root of \( N \) is recommended for a Kriging metamodel, where \( N \) is the number of sample points used to construct a metamodel. Some other references about Kriging in simulation can refer to (Koehler & Owen, 1996; Santner, Williams, & Notz, 2003; Liu & Smith, 2007; Baioumy, Liu, & Smith, 2008; Khafaji, Liu, & Smith, 2009).

The recent representative work of the Kriging applications to simulation interpolation is given by Kleijnen and van Beers (2003, 2004, 2005). Their work mainly focuses on three aspects:

1. Investigate the application of Kriging in stochastic simulation when the variances of simulation outputs are not constant, and show that Ordinary Kriging (OK) is a robust interpolation method and seems very insensitive to variance heterogeneity (Kleijnen & van Beers, 2005).
2. Propose a sequential and application-driven (customized) experimental design method based on Kriging for simulation interpolation (Kleijnen & van Beers, 2004). Kleijnen and van Beers demonstrate that the developed method can be applied to other types of metamodels and stochastic simulation, especially discrete event simulation. It is noted that although what they discuss is discrete-event simulation, the interpolated variables are still continuous.
3. Discuss the Kriging interpolation for stochastic simulation and develop Detrended Kriging (Van Beers & Kleijnen, 2004).
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