A Study on Improving Accuracy of Kriging Models by Using Correlation Model Selection and Penalized Log-Likelihood Function

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In this paper, two strategies are presented to improve the accuracy of Kriging models. Without sensitivity information, sampling-based methods are used in reliability-based design optimization (RBDO). In sampling-based RBDO, true models are often approximated by using surrogate models, since direct reliability evaluation requires evaluations at very large number of sample locations and true samples are computationally expensive in most practical applications. Since the Kriging model is accurate compared with other surrogate methods, it is widely used not only in geostatistics but also in engineering applications. The Kriging model is based on a Gaussian random process, which includes a spatial correlation function. To identify the best correlation function parameter for the given correlation function, maximum likelihood estimation (MLE) is widely used. However, MLE can be inaccurate when the sample size is small and samples are not close enough relatively to the spatial correlation length. In such situations, estimation of Kriging models may give either misleading results or flat predictions. Therefore, in literature, a penalized log-likelihood function is introduced to avoid such a wrong result by using a penalty function and cross-validation error. Authors of the original penalized log-likelihood function recommended using the Smoothly Clipped Absolute Deviation (SCAD) penalty function along with grid samples for the parameter λ of the penalty function. However, since the penalty amount of the SCAD penalty function is flat outside of a fixed region, the effect of the SCAD penalty function is relatively small compared with L1 penalty function and it is difficult to set up appropriate parameter value. Examples show that L1 penalty is more stable. The appropriate grid size for the parameter λ is depending on the target problem. Therefore, a small grid size is usually more stable and gives better performances. However, a small grid size increases the number of cross-validations rapidly to estimate. And when the sample size is relatively large, the influence of the penalty function is negligible. Therefore, pattern search algorithm is applied to find better λ starting from λ=0, where the penalty function is zero. Then the number of computations does not increase much with smaller tolerance for λ; and λ values will converge to zero rapidly when sample size is large. At the same time, some correlation function types are better than other correlation function types to describe the correlation structure of given data at samples. In geostatistics, correct correlation function type is identified first by drawing a variogram or a correlogram. However, such a graphical method is difficult to be applied for high-dimensional problems with directional tendency, because the number of figures to examine increases rapidly. Furthermore, it requires users some knowledge and understanding on the relationship between the data and variogram. In engineering field, the correlation function is often fixed as Gaussian or General Exponential functions, since they are differentiable and provides a relatively smooth surface. However, examples show that other correlation function type could yield better results. To select the best correlation function, maximum likelihood estimation can be applied. The proposed method is applied to mathematical and engineering examples and resulted in better output. The condition when the penalized-log likelihood function is beneficial is being investigated to minimized unnecessary calculations. If both penalized log-likelihood function and correlation function selection are combined and implemented, performances of Kriging models will be more stable and accurate.