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Importance of correlogram analysis for kriging metamodels

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Abstract : This paper presents correlogram analysis for kriging metamodels. Kriging metamodels have been used in simulation since 1989. Correlogram analysis is the core issue for kriging because the kriging weights are estimated using theoretical correlogram models. Model assumptions directly affect the covariogram and correlogram estimations. Correlogram estimation and fitted theoretical model selection must be done carefully before using in kriging metamodels. Correlogram analysis is shown on four test function. According to result there are valid experimental correlogram estimations for test functions which are considered in this study. Thus, theoretical correlogram model are able to be obtained. The experimental correlogram estimations have decreased rapidly as h increases for two and three dimensional functions and, have decreased slowly as h increases for eight dimensional functions considered in this study.

Keywords: Spatial correlation, variogram, covariogram, correlogram, kriging metamodels.

I.INTRODUCTION

Simulation models can be quite complex to conduct too many experiments, and a simplified model of these models can be developed with a simpler approach [1, 2, 3]. This model is called the metamodel and defined as “the model of the model”. Such models are used instead of simulation models for many purposes such as sensitivity analysis, observation of the change of inputs against change of inputs, and optimization [4]. There are many methods to obtain a metamodel. One of these methods is known as kriging [5].

Sacks et all. [5] firstly applied kriging to deterministic simulation models as a metamodel. Van Beers and Kleijnen [6] used kriging metamodel for stochastic simulation models. Later, Biles et al. [7] used the kriging metamodel in the constrained simulation optimization problem.

The kriging metamodels are the best unbiased estimators among all linear estimators and give the smallest mean squared error estimation [8, 6, 9]. The kriging metamodel gives a zero-estimation error for all the experimental points used in the kriging model [10, 9]. The kriging metamodels are more suitable for data obtained from large test areas [5, 8]. Kriging metamodels are equally compatible with linear and non-linear functions [8]. In addition, the kriging metamodels are an appropriate choice for many different and complex answer functions [11]. Kriging metamodels are flexible models because of the diversity of the correlogram model obtained from a sufficient number of examples [8, 11]. The metamodel obtained for a single set of parameters in the regression is used for all of the search space. The kriging metamodels recalculate each time by adapting their weights to the input variable at each forecast point [9]. Variogram analysis is the most important step in kriging as it is used to determine the kriging weights. [12, 13]. Corelogram is generally used instead of variograms in kriging metamodels for simulation [5, 14, 8, 6, 15].

In this study, correlogram analysis which is the most critical step of the kriging metamodels for the simulation models are examined. Correlogram analysis is strongly related with the model assumption of the random process. Clearly relationship between the input variables and output variables are so important to estimate experimental correlogram. Correlogram estimation and fitted theoretical model selection must be done carefully before using in kriging metamodels. According to result there are valid experimental correlogram estimates for test functions which are considered in this study. Thus, theoretical correlogram models have been able to be obtained. The experimental correlogram estimations have decreased rapidly as h increases for two and three dimensional test functions and, have decreased slowly as h increases for eight dimensional test functions.

In section 2, the variogram, covariogram and corelogram used in correlogram analysis are examined. In section 3, example applications are explained on the four test functions. In Section 4, the conclusions are presented.

II.CORRELOGRAM ANALYSIS

The spatial correlation is quantified by semi-variogram, shortly called the variogram [16]. Variogram estimation is the most important step of kriging as it is used to determine the kriging weights [12, 13]. The semi-variogram concept was first used by Matheron because it was calculated as half of the variance [16]. The value of the variogram continues to increase to a distance value called "range" as the distance value increases. If the variogram value for a distance value near zero is different from zero, this value is called "nugget-effect" [17].

Assuming that $Z(\mathbf{x})$ is a random process, D is the experimentation area and $\mathbf{x}$ is spatial point and $\mathbf{x} \in D$. $Z(\mathbf{x}) = \{z(\mathbf{x_1}), \dots, z(\mathbf{x_n})\}$ is the set of the experimental values of the random variable $Z(\mathbf{x})$ at the points $\mathbf{x}$. Where $\mathbf{x} = (x_1, \dots, x_k)'$ is input variable vector, $\mathbf{x_i} = (x_{1i}, \dots, x_{ki})'\ \forall\, i = 0, \dots, n$ is the i nth point vector and n is the number of experiments. The model assumptions for the $Z(\mathbf{x})$ process are given in (1) to (4):

$$Z(\mathbf{x}) = \mu(\mathbf{x}) + \varepsilon(\mathbf{x}) \tag{1}$$

$$E[Z(\mathbf{x})] = \mu(\mathbf{x}) \tag{2}$$

$$E[\varepsilon(\mathbf{x})] = 0 \tag{3}$$

$$\mathrm{Var}\big(Z(\mathbf{x})\big) = \sigma^2 = c(0) \tag{4}$$

2.1. Variogram

The variogram value between the observation values $Z(\mathbf{x_i})$, $Z(\mathbf{x_j})$ is calculated as in (5).

$$\gamma(\mathbf{x_i}, \mathbf{x_j}) = \frac{1}{2} E[\big(Z(\mathbf{x_i}) - Z(\mathbf{x_j})\big)^2] \tag{5}$$

In this study it is assumed that the variogram is isotropic: $\gamma(h) = \gamma(-h)$. Matheron [18] defined that a logical estimator of experimental variogram given in (6).

$$\hat{\gamma}(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} (Z(\mathbf{x_i}) - Z(\mathbf{x_i} + h))^2 \tag{6}$$

Where $N(h)$ is the number of pairs of $Z(x_i)$, $Z(x_i + h)$ and h is the distance between the experiments [16]. Cresssie and Hawkins [12] proposed a robust variogram estimator given in (7).

$$\hat{\gamma}(h) = \frac{1}{2} \left[\frac{1}{N(h)} \sum_{i=1}^{N(h)} \big(Z(\mathbf{x_i}) - Z(\mathbf{x_i} + h)\big)^{\frac{1}{2}}\right]^4 \Big/ \left(0.457 + \frac{0.494}{N(h)}\right) \tag{7}$$

2.2. Covariogram

The covariogram is calculated as given in (8) to (10).

$$\hat{c}(h) = \frac{1}{N(h)} \sum_{i=1}^{N(h)} (Z(\mathbf{x_i}) - \mu)\,(Z(\mathbf{x_i} + h) - \mu) \tag{8}$$

$$\mu = \frac{1}{n} \sum_{i=1}^{n} Z(\mathbf{x_i}) \tag{9}$$

$$\hat{\gamma}(h) = \sigma^2 - \hat{c}(h) \tag{10}$$

2.3. Correlogram

The correlogram is calculated as given in (11).

$$\hat{r}(h) = {}^{\hat{c}(h)}\!/_{\sigma^2} \tag{11}$$

Where $|\hat{r}(h)| \leq 1$. Correlogram values are used instead of variogram and covariogram to calculate kriging weights especially in deterministic simulation optimization. When calculation of the kriging weights for each point, we need a theoretical correlogram model. Theoretical correlogram model must fit to the experimental correlogram. General correlogram model is given in (12). The mostly used theoretical correlation models in the literature are given in Table 1 [5, 14, 15]. Where, θ_i, pi and θ are the model parameters.

$$r(h) = \exp\big(-\sum_{i=1}^{k} (\theta_i h_i)^{p_i}\big) = \prod_{i=1}^{k} \exp\,(-(\theta_i h_i)^{p_i}\,) \tag{12}$$

Table 1. Theoretical correlogram models

Model name	Model
Gaussian	$r(h) = \exp\,(-({}^{h}/_{\theta})^2)$
Exponential	$r(h) = \exp\,(-{}^{h}/_{\theta})$
Linear	$r(h) = \max\,(1 - \theta h, 0)$
Mathern 1	$r(h) = \exp\,(1 - \theta h)\left(1 + \theta h + {}^{\theta^2 h^2}/_{3}\right)$
Mathern 2	$r(h) = \exp\,(-\theta h)\,(1 + \theta h)$

2.4. Parameter estimation

Two approaches are available in the literature to estimation for the parameters of the theoretical correlogram model family given in the Table 1. First method is the maximum likelihood estimation [5, 9, 7]. Second method is least square estimation (LSE) and variants [7]. In this study LSE approach preferred because the spatial statistician mostly used this approach. Estimation of the correlogram model parameter is obtained as given in (13). Where, $\hat{\theta}$ is the estimation of the θ.

$$\hat{\theta} = \arg\min_{\theta} (\hat{r}(h) - r(h))^2 \tag{13}$$

2.5. Some important remarks on experimental correlogram estimation

The model assumptions are very important to estimate the experimental correlogram in (11). Three cases may be in the assumptions.

i. $E[Z(\mathbf{x})] = \mu(\mathbf{x}) = \mu$ is constant and known, then $\hat{r}(h)$ can be calculated directly using the (11) with the (8) because the mean of the process is calculated as in (9).

ii. $E[Z(\mathbf{x})] = \mu(\mathbf{x}) = \mu$ is constant and unknown, then $\hat{r}(h)$cannot be calculated directly using (11) because the mean of the process given in (9) is not calculated. It is needed to use variogram estimations given in (6) or (7). Then $\hat{r}(h)$ can be calculated using the (11) with the (10) because the mean of the process is not needed.

iii. $E[Z(\mathbf{x})] = \mu(\mathbf{x})$ is function of **x** then $\hat{r}(h)$ can be calculated as discussed in (ii).

Only simple kriging model assumes that the mean of the process is constant and known. Ordinary kriging model assumes that the mean of the process is constant and unknown. Universal kriging models assume that the mean of the process is a function of inputs [17].

III. EXAMPLE APPLICATIONS

Four test functions given in the Table 2 are used for correlogram analysis in this study. Latin hypercube design (LHD) is used to obtain training data sets. LHD was first described for computer experiments by McKay et al. [19]. LHD is produced by dividing each factor column into n equal intervals and permuting each column randomly [20]. Training data sets are including 26, 28, 72 and 72 experiments for Zettl, Ishigami, Zakharov and Brown functions respectively.

Table 2. Test function

Function name	Function
Zettl	$f(x) = 0.25x_1 + (x_1^2 - 2x_1 + x_2^2)^2$ $-5 \leq x_1, x_2 \leq 10$
Ishigami	$f(x) = \sin(x_1) + 0.7\sin^2(x_2) + 0.1x_3^2\sin(x_1)$ $-\pi \leq x_i \leq \pi, \quad 1 \leq i \leq 3$
Zakharov	$f(x) = \sum_i^8 x_i^2 + (\sum_i^8 0.5x_i)^2 + (\sum_i^8 0.5ix_i)^4$ $-5 \leq x_i \leq 10, \quad 1 \leq i \leq 8$
Brown	$f(x) = \sum_i^7 (x_i^2)^{(x_{i+1}^2+1)} + (x_{i+1}^2)^{(x_i^2+1)}$ $-1 \leq x_i \leq 4, \quad 1 \leq i \leq 8$

Figure 1, Figure 3, Figure 5 and Figure 7 shows experimental variogram estimates and theoretical variogram model plots for Zettl, Ishigami, Zakharov and Brown functions respectively. And, Figure 2, Figure 4, Figure 6 and Figure 8 shows MSE (mean squared error) of theoretical variogram models' performances for Zettl, Ishigami, Zakharov and Brown functions respectively.

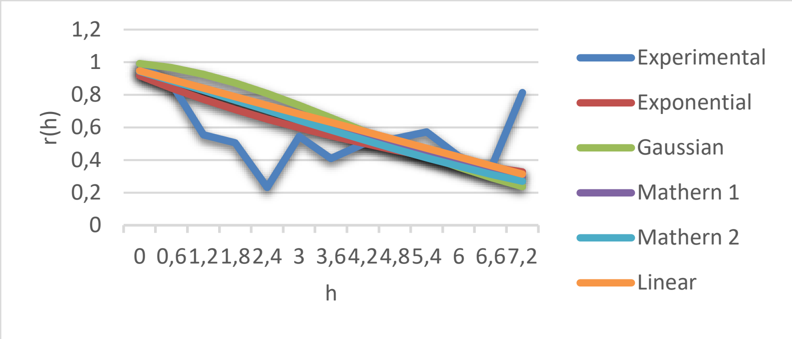

Figure 1. Correlogram for Ishigami function

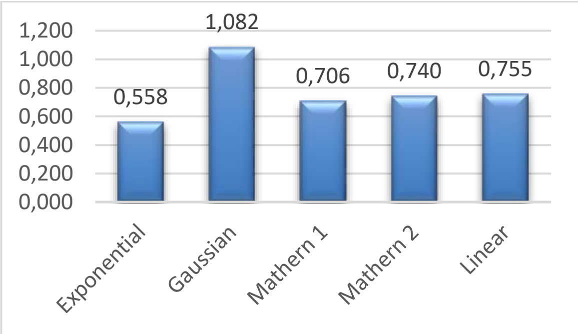

Figure 2. MSE of theoretical correlogram models for Ishigami function

Figure 1 shows that experimental correlogram estimations, r(h), decrease as h increases. This means that there are valid experimental correlogram estimations and theoretical correlogram model for Ishigami function. Exponential correlogram model which has the smallest MSE among all theoretical correlogram models given in Figure 2 is chosen to use.

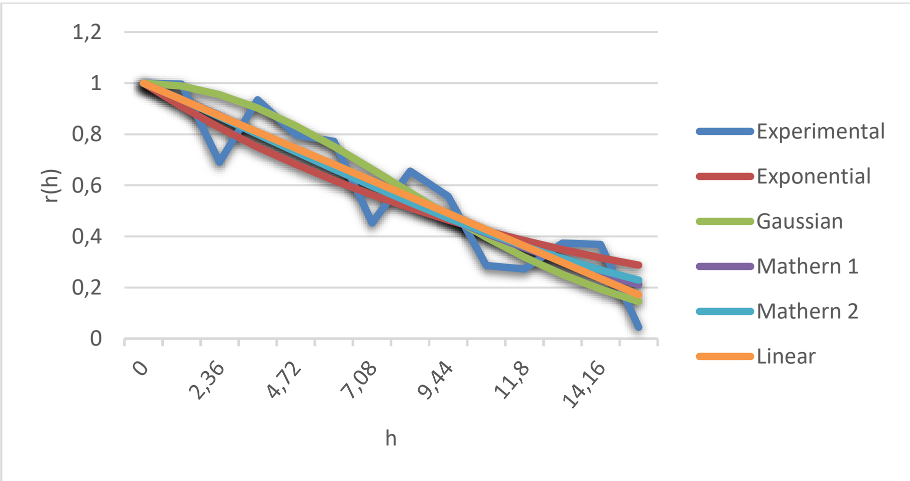

Figure 3. Correlogram for Zettl function

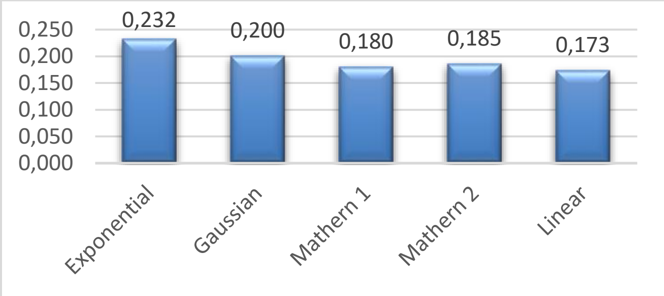

Figure 4. MSE of theoretical correlogram models for Zettl function

Figure 3 shows that experimental correlogram estimations, r(h), decrease rapidly as h increases. This means that there are valid experimental correlogram estimations and theoretical correlogram model for Zettl function. Mathern 1 correlogram model which has the smallest MSE among all theoretical correlogram models given in Figure 4 is chosen to use.

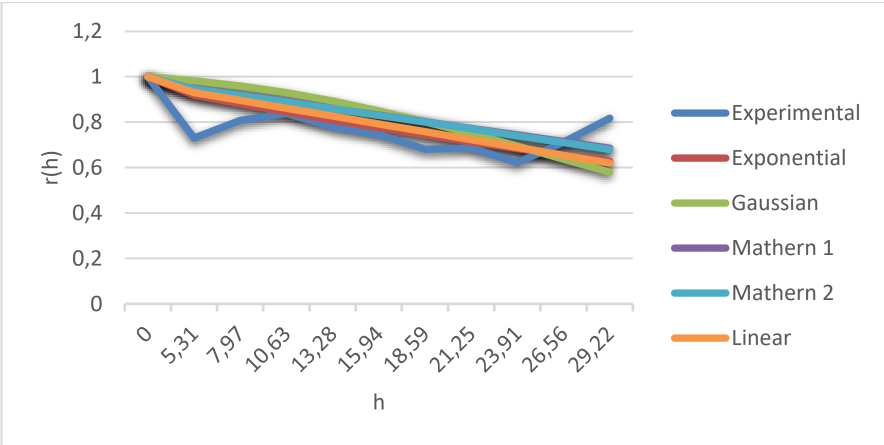

Figure 5. Correlogram for Zakharov function

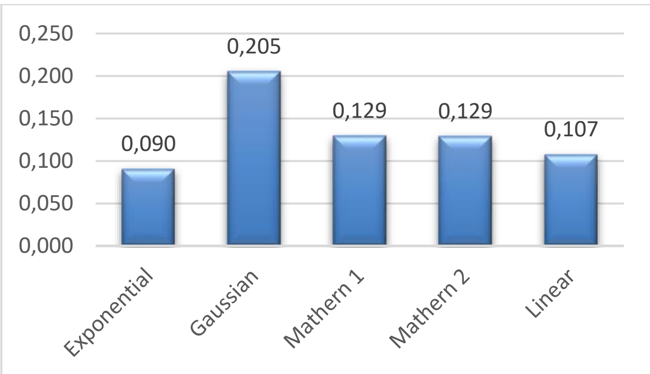

Figure 6. MSE of theoretical correlogram models for Zakharov function

Figure 5 shows that experimental correlogram estimations, r(h), decrease slowly as h increases. This means that the spatial correlation is very high as h increases and there are still valid experimental correlogram estimations and theoretical correlogram model for Zakharov function. Exponential correlogram model which has the smallest MSE among all theoretical correlogram models given in Figure 6 is chosen to use.

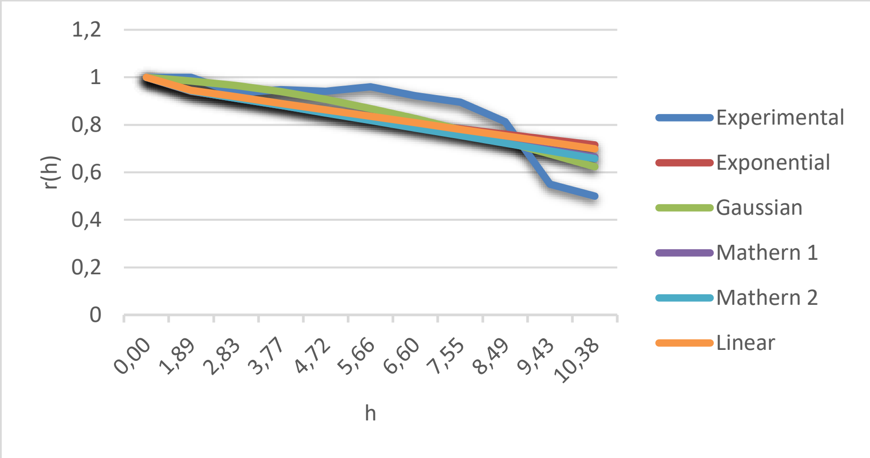

Figure 7. Correlogram for Brown function

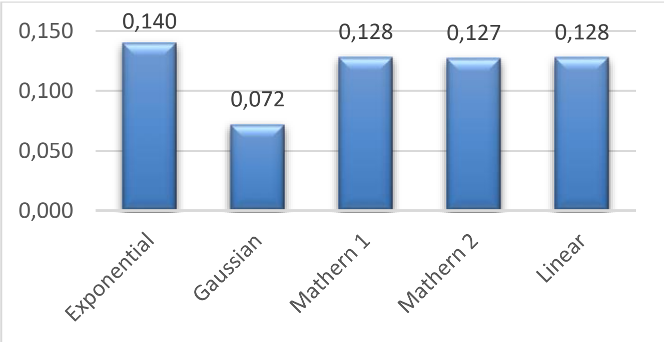

Figure 8. MSE of theoretical correlogram models for Brown function

Figure 7 shows that experimental correlogram estimations, r(h), decrease slowly as h increases. This means that the spatial correlation is very high as h increases and there are still valid experimental correlogram estimations and theoretical correlogram model for Brown function. Gaussian correlogram model which has the smallest MSE among all theoretical correlogram models given in Figure 8 is chosen to use.

The experimental correlogram estimations have decreased rapidly as h increases for two and three dimensional test functions and, have decreased slowly as h increases for eight dimensional test functions.

IV.CONCLUSION

Correlogram analysis is strongly related with the model assumption of the random process. And correlogram models directly affect the weights of kriging metamodel. Correlogram can be estimated based on covariogram for simple kriging because the model assumes that the mean of the process is constant and known. Correlogram can be estimated based on variogram for ordinary kriging and universal kriging because the model assumes that the mean of the process is constant, and unknown and a function of input variables, respectively. Because of these remarks, correlogram estimation and fitted theoretical model selection must be done carefully. Another point to be taken in to account that the correlogram estimation must be feasible for the computer experiments, since the input variable dimension is usually much larger than two or three.

According to result there are valid experimental correlogram estimates for test functions which are considered in this study. Thus theoretical correlogram models have been able to be obtained. The experimental correlogram estimations have decreased rapidly as h increases for two and three dimensional functions and, have decreased slowly as h increases for eight dimensional functions. If the simulation has more than one output variables each output must be analyzed separately because the theoretical correlogram model could be different.

Future work will be on the non-isotropic variogram/correlogram analysis for high dimensional problem and its effect on predictions.

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