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UNCERTAINTY QUANTIFICATION OF MULTIVARIATE GAUSSIAN PROCESS REGRESSION FOR APPROXIMATING MULTIVARIATE COMPUTER CODES

YOUNUS AL-TAWEEL[1], §

Abstract. Gaussian process regression (GPR) models have become popular as fast alternative models for complex computer codes. For complex computer code (CC) with multivariate outputs, a GPR model can be constructed separately for each CC output, ignoring the correlation between the different outputs. However, this may lead to poor performance of the GPR model. To tackle this problem, multivariate GPR models are used for complex multivariate deterministic computer codes. This paper proposes measures for quantifying uncertainty and checking the assumptions that are proposed in building multivariate GPR models. For comparison, we also constructed a univariate GPR model for each CC output to investigate the effect of ignoring the correlation between the different outputs. We found that the multivariate GPR model outperforms the univariate GPR model as it provides more accurate predictions and quantifies uncertainty about the CC outputs appropriately.

Keywords: multivariate Gaussian process, measures, multivariate deterministic computer codes.

AMS Subject Classification: 83-02, 99A00

1. Introduction

Simulations have become popular methods for investigating real-world systems. This simulation is achieved via a complex computer code (CC) which is a mathematical representation of a real system. Complex CCs, however, can be time-consuming and so running the CC can only be done at a fixed number of runs. Statistical models have become a practical solution for tackling the time-consuming problem of CCs. The outputs of CC are considered to be realizations of a random process. The Bayesian framework is used to construct a probability distribution, called Gaussian process regression (GPR) model, that can be conducted to obtain approximations of the CC outputs and for uncertainty quantification of its outputs.

GPR models are statistical techniques that have been applied in a variety of sectors in science and technology. In engineering modeling, for example, [1] used GPR models for accounting for the uncertainty of a design of an infantry fighting vehicle. [2] built

[1] University of Mosul, College of Education for Pure Science, Department of Mathematics, Iraq.
e-mail: younus.altaweel@uomosul.edu.iq; ORCID: https://orcid.org/0000-0001-7167-8079.

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a GPR model to quantify the uncertainty of bridge model outputs. [3] used a GPR model to obtain approximations of an engine shaft horsepower. In climate modeling, [4] used a GPR model for a global aerosol to provide sensitivity analysis for unknown parameters. [5] interpolated outputs of model for Earth Climate System. [6] used a GPR model for inferring a background ocean vertical diffusivity parameter in climate models. [7] quantified the contributions of remote and local black carbon emissions to its concentrations using GPR models.

In environment modeling, [8] performed a global sensitivity analysis using GPR models for remotely based vegetation indices. [9] used GPR models to provide approximations of a land biosphere model. [10] investigated the performance of GPR models for modeling wildland fire emissions. In health modeling, [11] used regression models to reduce the time for running computationally expensive health economic models. [12] used a GPR model for a gravity model to make inferences for the Spatio-temporal dynamics of infectious diseases. [13] constructed a GPR model for complex infection disease models. The GPR model was used by [15] to provide variance-based sensitivity indices of a cardiac cell model. In deterministic computer modeling, the GPR model was used by [14] with computationally unstable correlation matrices to interpolate deterministic CCs. [16] used GPR models to solve boundary value problems. [17] used the GPR model for uncertainty quantification based on the lower bound error of the regression model.

In several areas, however, complex CCs may have multiple outputs. Univariate GPR models can be built separately for each output of the CC, ignoring the correlation between the outputs. This may not capture information between the outputs. To solve this problem, a multivariate GPR model can be used for complex multivariate CCs to model the outputs jointly. Multivariate GPR models take into account the correlation between the outputs. In this work, we propose some measures for checking the assumptions that are used in constructing multivariate GPR models as surrogates for multivariate deterministic CCs. Using the proposed measures, the performance of the multivariate GPR models with that of univariate GPR models is compared for each CC output.

The following is the order of the paper. In Section 2, we presents the concept of multivariate GPR models for multivariate CCs. In Section 3, the procedure of constructing multivariate regression models is explained. Section 4 reviews designs for generating training and test points. In Section 5, various measures for validating multivariate regression models. In Section 6, multivariate regression models are applied to some multivariate CCs examples. Finally, in Section 7, the conclusion is given.

2. Multivariate GPR model

Univariate GPR models were first used by [18] where they provide the process of constructing a GPR model for one output CC. Then, GPR models have been used widely under a Bayesian framework. Modern applications of complex CCs tend to have multiple outputs. A generalization of multiple univariate GPR models is known as a multivariate GPR model. Multivariate GPR models deal with CCs that have more than one output. For simplicity, one can construct a GPR model for each output of the multivariate CC separately, ignoring the correlation between outputs. However, the outputs of multivariate CCs may not be independent and therefore, the results may not be accurate. To consider the structure in the model outputs, multivariate GPR models can be used for multivariate CCs to obtain more accurate results than using a univariate GPR model for each output.

The multivariate to the Gaussian process (GP) was considered in different ways. For example, [19] generalized univariate GPR models to matrix Gaussian with a column covariance matrix with a separable covariance function and a row covariance matrix that is considered as an extra hyperparameter. [20] used principal components for the dimensional reduction of a multivariate output CC. They assumed the principal components to be independent. [21] built a GPR model using the between-output metric. He presented a method that considers a Cartesian grid for constructing GPR model for the multidimensional outputs of the CC.

These methods, however, suffer from the problem of separability of the covariance matrix that implies the same roughness parameters for each output. This may not be suitable, for example, for multivariate CCs that have different types of outputs as the correlation functions will not be accurately specified. In order to allow the roughness parameters to be varied, a nonseparable covariance matrix has been used. For example, [22] showed that for two positive definite covariance functions, the convolution matrix is positive definite. [23] constructed a multivariate GPR model for a CC that simulates multiple types of outputs simultaneously. They presented a nonseparable covariance function using the convolution approach. They used two methods to construct a nonseparable covariance function, coregionalization models and convolution methods.

In this work, we investigate the performance of measures for validating multivariate GPR models. [24] developed a graphical method, called the coverage interval (CI), that can be used to evaluate the number of test outputs that are within the of $(1-\alpha)100\%$ intervals. The CI measure can be used to find the proportion of the test outputs that are within the $(1-\alpha)100\%$ intervals with multiple values of $(1-\alpha)$. Thus, it tests the Gaussian assumption in building GPR models. [24] investigated the performance of the CI measure for univariate GPR models. Therefore, we develop and extend the CI measure for multivariate GPR models. For comparison, we also construct a GPR model for each output of the CC and see the effect of ignoring the correlation between the different outputs. For additional confirmations, we apply some other measures to see the performance of multivariate GPR models.

3. Building multivariate GPR model

In this section, we review an approach, given by [25], for constructing the multivariate GPR model. This case of the multivariate GPR model is computationally tractable. Suppose we have a multivariate CC, $\mathbf{f}(\cdot):\chi\to\mathbb{R}^k$, of input, $\mathbf{x}\in\chi\to\mathbb{R}^p$ and produces a output $\mathbf{y}\in\mathbb{R}^k$, where $k>1$, p is the dimension of the input. The function $\mathbf{f}(\cdot)$ is considered to be an unknown. The uncertainty is represented by the Gaussian process conditional on parameters.

Let $\mathbf{X}^{(r)}=(\mathbf{X}_1,\ldots,\mathbf{X}_{n_r})$, where n_r is the set of input points, and $r\leq k$ are observations of kind r and therefore, the $\mathbf{X}^r_{[n_r\times p]}$ is the design matrix for the observations of kind r. Thus, in the multivariate GPR model, k different kinds of observations exists, $f_r(\cdot)$, for $r=1,\ldots,k$. Each of which follows a GP

$$\mathbf{f}(\cdot)|\boldsymbol{\beta},\boldsymbol{\Sigma},\mathbf{r}\sim N_k(\mathbf{m}(\cdot),\mathbf{c}(\cdot,\cdot)\boldsymbol{\Sigma}). \tag{1}$$

The mean function is given by a linear function

$$\mathbf{m}(\mathbf{x})=\mathbf{H}\boldsymbol{\beta} = \begin{pmatrix}\mathbf{h}_1(\mathbf{X}^1)^T & 0 & \cdots & 0\\ 0 & \mathbf{h}_2(\mathbf{X}^2)^T & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & \mathbf{h}_k(\mathbf{X}^k)^T\end{pmatrix}\begin{pmatrix}\beta_1\\ \beta_1\\ \vdots\\ \beta_k\end{pmatrix}, \tag{2}$$

where $\mathbf{h}_r(\cdot)$ are the regression functions, $h_1(\mathbf{x}), \ldots, h_q(\mathbf{x})$, for the kind r of the observations. Therefore, the generalized regressor matrix is $\mathbf{H}_{[\sum_{r=1}^{k} n_r \times \sum_{r=1}^{k} q_r]}$. The $\boldsymbol{\beta} = (\beta_0, \ldots, \beta_k)$ is a vector of coefficient parameters.

The covariances between the different kinds of the observations, $r \neq s$, is given by $\mathrm{Cov}(f_r(\mathbf{x}), f_s(\mathbf{x}')) \neq 0$ where $f_r(\mathbf{x})$ and $f_s(\mathbf{x}')$ are outputs of the inputs $\mathbf{x}$ and $\mathbf{x}'$ at the observations kind r and s. Thus, the covariance matrix is given by

$$\boldsymbol{\Sigma} = \begin{pmatrix} \Sigma^{(11)} & \Sigma^{(12)} & \ldots & \Sigma^{(1k)} \\ \Sigma^{(21)} & \Sigma^{(22)} & \ldots & \Sigma^{(2k)} \\ \vdots & \vdots & \ddots & \vdots \\ \Sigma^{(k1)} & \Sigma^{(k2)} & \ldots & \Sigma^{(kk)} \end{pmatrix}. \tag{3}$$

The covariance between different outputs, kinds r and s, at any input point is determined by $\Sigma^{(rs)}$. The covariance function depends on k positive correlation parameters $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_k)$.

The Σ in equation (3) is formulated such that $\Sigma^{(rr)}$ to be determined by standard methods from univariate analysis, using

$$\mathrm{Cov}(f_r(\mathbf{x}), f_r(\mathbf{x}')) = \sigma^2 C(\mathbf{x}, \mathbf{x}'), \tag{4}$$

where the elements i, jth of $C(\mathbf{x}, \mathbf{x}')$ is the covariance between the i output when it is run at input x and the j when run at input x. The covariance function is given as $C_{rs}(\mathbf{x}, \mathbf{x}') = \mathrm{Cov}(f_r(\mathbf{x}), f_s(\mathbf{x}'))$. Thus, we have $\Sigma^{(rs)} C_{rs}(\mathbf{X}^r, \mathbf{X}^s)$ as the matrix of covariances between the r kind of observations and the kind s observations, i.e. between $f_r(\mathbf{X}^r)$ and $f_s(\mathbf{X}^s)$.

The multivariate covariance structure Σ^{rs} must be positive definite in which Σ in equation (3) must be positive definite for $\mathbf{X}^1, \mathbf{X}^2, \ldots, \mathbf{X}^k$. The $C_{rs}(t) = C_{rs}(\mathbf{x} - \mathbf{x}')$ is a matrix and it is given by the formula

$$C_{rs}(t) = \int_{w \in \mathbb{R}^q} e^{iw^T t} dF_{rs}(w), \tag{5}$$

where $F_{rs}(w)$ is a positive definite matrix. For every w, $|f(w)|$ is utilized for the matrix containing the entry (r, s), and it must be positive definite. The general form with $k = 3$ for illustration is

$$\|g(w)\| = \begin{pmatrix} G_1 & 0 & 0 \\ 0 & G_2 & 0 \\ 0 & 0 & G_3 \end{pmatrix}. \tag{6}$$

where $G_1 = \frac{\exp[-\frac{1}{2}\mathbf{w}^T \mathbf{S}_1^{-1} \mathrm{w}]}{|2\pi \mathbf{S}_1|^{1/2}}$, $G_2 = \frac{\exp[-\frac{1}{2}\mathbf{w}^T \mathbf{S}_2^{-1} \mathrm{w}]}{|2\pi \mathbf{S}_2|^{1/2}}$ and $G_3 = \frac{\exp[-\frac{1}{2}\mathbf{w}^T \mathbf{S}_3^{-1} \mathrm{w}]}{|2\pi \mathbf{S}_3|^{1/2}}$. In practice we choose C($\mathbf{t}$)=exp $-\mathbf{t}^T \mathbf{B} \mathbf{t}$ where $\mathbf{B} = \frac{\mathbf{S}^{-1}}{2}$. This gives $\mathrm{Cov}(f_r(\mathbf{x}), f_r(\mathbf{x}')) = \sigma^2 C(\mathbf{x}, \mathbf{x}') = \exp -\mathbf{t}^T \mathbf{B} \mathbf{t}$. This ensures that the matrix$\mathbf{S}_i$ are positive definite.

In order to account for nonzero covariances between the different kinds of observations, a positive semi-definite matrix is used

$$\|f(w)\| = \begin{pmatrix} G_1 & G_{1.2} & G_{1.3} \\ G_{2.1} & G_2 & G_{2.3} \\ G_{3.1} & G_{3.2} & G_3 \end{pmatrix}, \tag{7}$$

where $G_{1.2} = G_{2.1} = \frac{\exp[-\frac{1}{2}\mathbf{w}^T (\frac{1}{2}\mathbf{S}_1^{-1} + \frac{1}{2}\mathbf{S}_2^{-1}) \mathrm{w}]}{|2\pi \mathbf{S}_1|^{1/4} \cdot |2\pi \mathbf{S}_2|^{1/4}}$, $G_{1.3} = G_{3.1} = \frac{\exp[-\frac{1}{2}\mathbf{w}^T (\frac{1}{2}\mathbf{S}_1^{-1} + \frac{1}{2}\mathbf{S}_3^{-1}) \mathrm{w}]}{|2\pi \mathbf{S}_1|^{1/4} \cdot |2\pi \mathbf{S}_3|^{1/4}}$, $G_{2.3} = G_{3.2} = \frac{exp[-\frac{1}{2}\mathbf{w}^T (\frac{1}{2}\mathbf{S}_2^{-1} + \frac{1}{2}\mathbf{S}_3^{-1}) \mathrm{w}]}{|2\pi \mathbf{S}_2|^{1/4} \cdot |2\pi \mathbf{S}_3|^{1/4}}$. The product of a positive semi-definite matrix and a positive definite matrix is a positive definite

$$C'_{rs}(\mathbf{t}) = M_{rs}C_{rs}(\mathbf{t})$$

where $M_{[k\times k]}$ is to account for the covariance between the different kinds of observations. The possibility of using other forms of the covariance function, in equation (7) is discussed by [25]. By integrating $\boldsymbol{\beta}$ out, we will have

$$\mathbf{f}(\cdot)|\mathbf{y},\boldsymbol{\theta} \sim GP_k\left(\mathbf{m}^{\ddagger}(\cdot),\mathbf{C}^{\ddagger}(\cdot,\cdot)\right) \tag{8}$$

so that for new observations $X^\star = (x_1^\star,\ldots,x_n^\star)$, we obtain the posterior mean $\mathbf{m}^{\ddagger}(X^\star)$ and the posterior covariance $\mathbf{C}^{\ddagger}(X^\star,X^\star)$ as

$$\begin{aligned} \mathbf{m}^{\ddagger}(X^\star) &= \mathbf{H}(X^\star)\hat{\boldsymbol{\beta}} + \mathbf{F}(X^\star)\mathbf{V}^{-1}(\mathbf{y}-\mathbf{H}\hat{\boldsymbol{\beta}}) && (9)\\ \mathbf{C}^{\ddagger}(X^\star,X^\star) &= \mathbf{C}(X^\star,X^\star) - \mathbf{F}(X^\star)\mathbf{V}^{-1}\mathbf{F}(X^\star)^T && (10)\\ &+ (\mathbf{H}(X^\star)-\mathbf{F}(X^\star)\mathbf{V}^{-1}\mathbf{H})(\mathbf{H}\mathbf{V}^{-1}\mathbf{H})(\mathbf{H}(X^\star)-\mathbf{F}(X^\star)\mathbf{V}^{-1}\mathbf{H})^T, \end{aligned}$$

where $\hat{\beta} = \left(\mathbf{H}\mathbf{V}^{-1}\mathbf{H}\right)^{-1}\mathbf{H}\mathbf{V}^{-1}\mathbf{y}$, $\mathbf{F}(X^\star) = \mathbf{C}(X^\star,X)$, $\mathbf{H} = \mathbf{I}_k\otimes\mathbf{h}(X)$ and $\mathbf{V} = \mathbf{C}(X,X)$. In order to remove the conditioning on $\boldsymbol{\theta}$, they are estimated, $\hat{\boldsymbol{\theta}}$ and treated as known instead of the true value $\boldsymbol{\theta}$, ignoring the uncertainty.

3.1. **Estimating the hyperparameters.** The scaler variance σ^2 in the univariate GPR model can be generalized to a positive definite $M_{k\times k}$. The $M_{k\times k}$ represents the covariances between the different kinds of observations. Then, the next steps are conditional on the roughness parameters and the matrix M. Thus, the roughness parameters are estimated first for each kind of observations separately. Then, the marginal variances are computed analytically for the posterior mode to be the diagonal of the matrix M. Finally, the off-diagonal of the matrix M is estimated using the determination of the posterior mode. A flat prior may be used to ensure positive definiteness. This procedure for estimating the hyperparameters works well in practice [25].

4. Design of experiment

To generate the training and test points, the maximin Latin hypercube design (maximin LHD) is used, which is based on distances between the input points [26]. The minimum distance is first calculated between the points. After that we choose the design which maximizes the minimum distance, i.e. the observations are generated as

$$\mathbf{X} = \max_{\mathbf{X}\subset\Omega}\ \min_{\{x,x'\}\in\mathbf{X}} dis(x_i,x_j). \tag{11}$$

5. Measures for validating multivariate GPR models

In this section, we use some measures for investigating the performance of multivariate GPR models. The first measure accounts the number of test outputs that are in $100\alpha\%$ intervals. Thus, it is used to check the normality in GPR model. This measure is obtained by

$$CI = \frac{1}{n^\star}\sum_{i=1}^{n^\star}\mathbf{1}(\mathbf{y}_i^\star \in CI_i(\alpha)). \tag{12}$$

The $\mathbf{1}$ represents the indicator function and $\mathbf{y}_i^\star$ is the test output. The observed value for CI is expected to be close to α. The CI reference distribution can be found using simulation as the CC outputs are correlated. We generate a large sample by a multivariate t distribution with $n-q$ degree of freedom (d.f.), $\mathbf{m}^{\ddagger}(X^\star)$ and $\mathbf{C}^{\ddagger}(X^\star,X^\star)$, and then, the CI is calculated.

The individual standardized errors (ISE) is another measure that we used. It is calculated as

$$\text{ISE} = \frac{\mathbf{y}_i^\star - \mathbf{m}^\ddagger(X^\star)}{\sqrt{\mathbf{C}^\ddagger(X^\star, X^\star)}}, \tag{13}$$

The ISE depends on the differences between the GPR predicted points and the CC outputs which are standardized using the squared root of the GPR variance. The errors of ISE measure should be between -2 and 2 if the GPR model is valid. Thus, if large ISE values are found, then the GPR model will not be valid and so the GPR predictions will not be accurate.

6. Illustrative Example for Multivariate CC

In this section, we investigate the development of some measures for validating multivariate GPR models. For comparison, we also construct GPR model for each output of the multivariate CC separately and see the accuracy of both models. We consider an example to see the performance of the proposed measures. Consider a multivariate CC given by

$$y_1 = \sin(5(x_1 + x_2)) + \cos(20(x_1 - x_2)) \tag{14}$$

$$y_2 = 4\sin(5(x_1 + x_2)) + 7(x_1 - x_2). \tag{15}$$

Thus, we have two input variables and two outputs. The y_1 and y_2 are chosen to be correlated. We selected 30 training inputs for the first function and 20 training inputs for the second function in the interval $[0, 1]^2$ using maximin LHD. Then, we obtained CC outputs at these training inputs. We will denote the outputs by $\mathbf{y} = (y_1, y_2)$. For validating the GPR models, we generated $n^\star = 20$ test points by maximin LHD and run the CC at these test points.

6.1. The Coverage Interval (CI) Measure.

After obtaining multivariate GPR models and univariate GPR models, we calculated the CI measure with different values of α for each test output. We generated 1000 sampled of 20 test outputs from multivariate t distribution with $n-k$ d.f., $\mathbf{m}^\ddagger(X^\star)$ and $\mathbf{C}^\ddagger(X^\star, X^\star)$. Then, we obtained simulated values of CI measure using equation (12). Figure 1 shows the observed CI values and their simulated mean values for the univariate and multivariate GPR models of the output 1, equation (14).

The left plot in Figure 1 shows the CI measure for univariate GPR model of the first output. It is indicated that most of the observed CI values are not close to the simulated mean values. Moreover, many of observed CI values are not within the 95% intervals. The right plot in Figure 1 shows the CI measure for the multivariate GPR model of the first output. It is shown that the observed CI values are so close to the simulated mean values. Furthermore, all the observed CI values are within the 95% intervals.

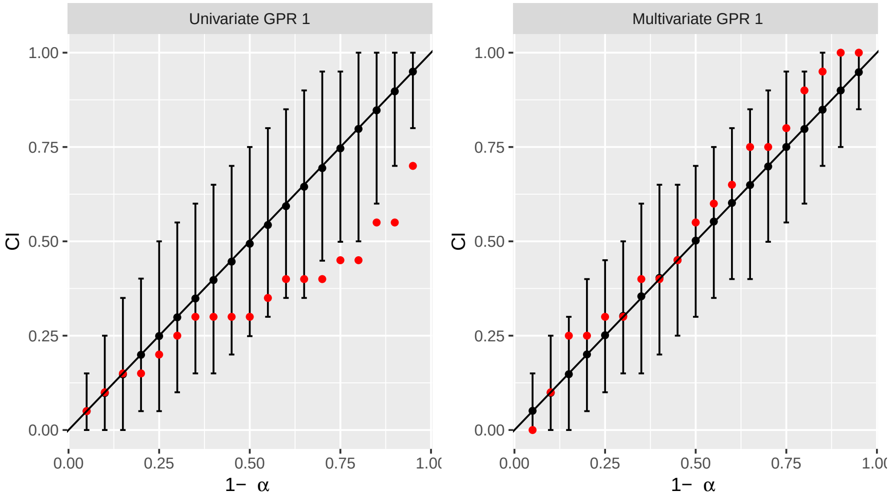

FIGURE 1. The observed CI values (red points) and simulated mean values (black points), for the univariate and multivariate GPR models of the output 1, equation (14), against different values of $(1-\alpha)$. The plots indicate that the normality is not suitable for the univariate GPR model of the first output.

Figure 2 shows the observed CI values and simulated mean values for the univariate and multivariate GPR models of the output 2, equation (15).

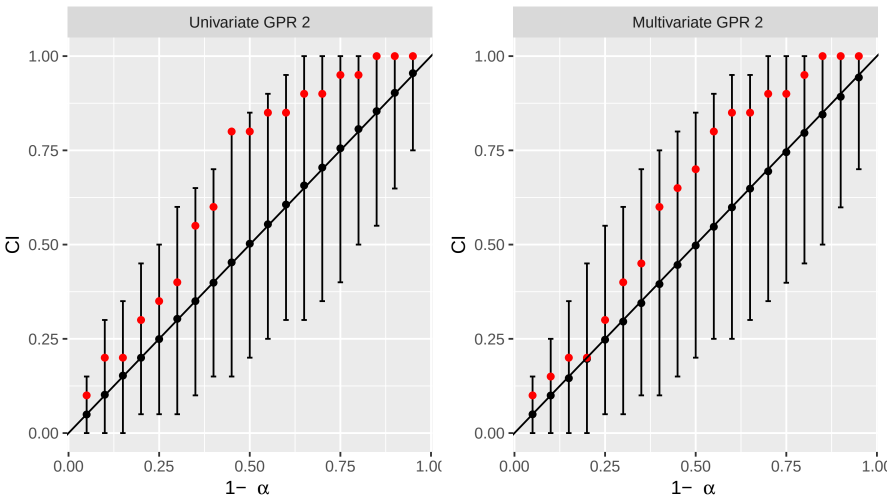

FIGURE 2. The observed CI values and the simulated mean values for the univariate and multivariate GPR models of the output 2, equation (15). The plots indicate that the normality is suitable for the univariate and multivariate GPR models.

It is indicated that many observed CI values for univariate GPR model are far away from the simulated mean values. However, all observed CI values are within the 95% intervals. This indicates that the normality is reasonable for constructing GPR models. The right plot is for the multivariate GPR model. It can be indicated that all the 95% intervals contain the observed CI values with the majority of the observed CI values are closer to the simulated mean values, indicating that the normality is reasonable for constructing GPR models.

6.2. **The Individual Standardized (ISE) Errors.** We also calculated the ISE, equation (13) for the univariate and multivariate GPR models. Thus, we plotted the ISE to investigate the performance of univariate and multivariate GPR models. Figure 3 presents the ISE for the univariate and multivariate GPR models of the output 1, equation (14).

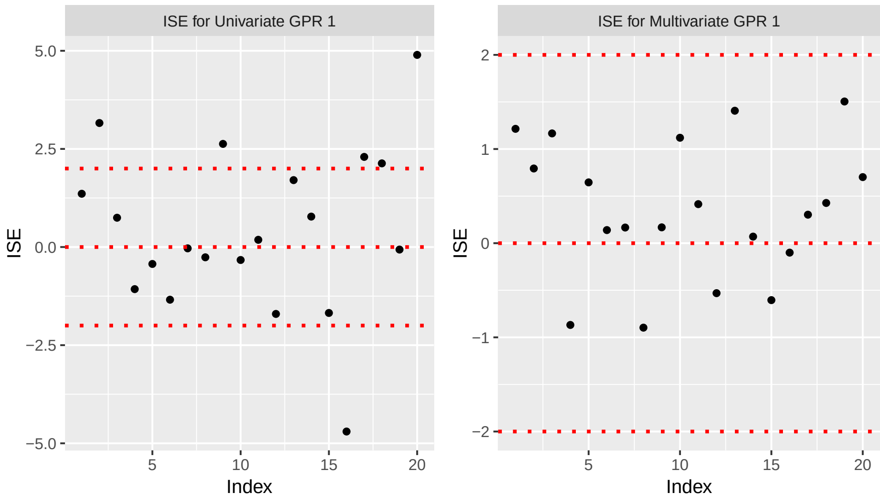

FIGURE 3. The ISE for the univariate and multivariate GPR models of the output 1, equation (14). The univariate GPR model produces Large values of ISE.

In Figure 3, the ISE values for the univariate GPR model of the output 1, equation (14) are presented in the left plot. It can be seen that there are several large values of ISE. The ISE values for the multivariate GPR model of the output 1, equation (14) are presented in the right plot. It can be shown that all the ISE lie in the bound seen in the plot.

Figure 4 shows the ISE for the univariate and multivariate GPR models of output 2, equation (15). The ISE values for the univariate GPR model of the output 2, equation (15) are presented in the left plot. It is indicated that although most of the ISE are small, there are several large ISE that lie outside the bounds. The ISE for the univariate GPR model of output 2, equation (15) are presented in the right plot. It can be shown that all the ISE are within the bound.

It can be concluded that the GPR model may not perform well when modeling it separately using univariate models. The performance GPR model that is modeled using multivariate models can perform better as they account for the correlation between the different outputs.

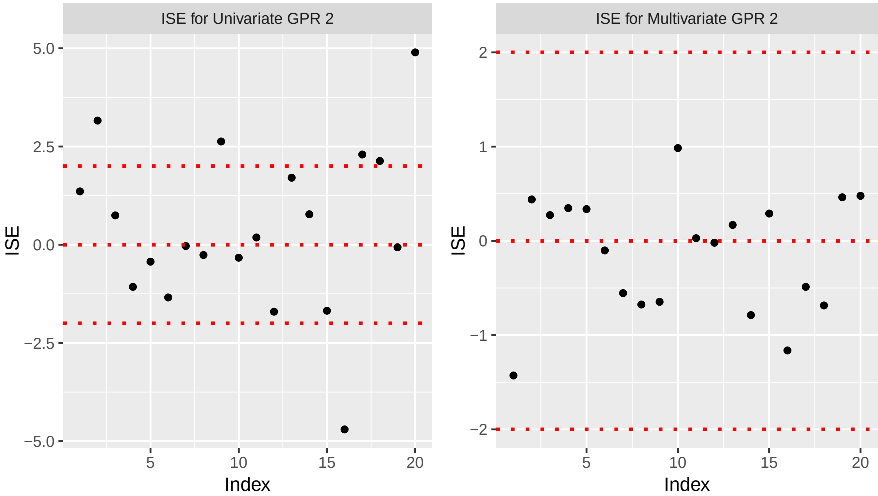

FIGURE 4. The ISE the univariate and multivariate GPR models of the output 2, equation (15). There are many large ISE for the univariate GPR model.

7. Conclusion

We have developed measures for quantifying uncertainty and investigating the performance of the multivariate GPR models as surrogates for multiple computer codes. Our measure is able to check if the multivariate normal assumption is reasonable for constructing multivariate GPR models or not. We have also compared the performance of multivariate GPR models with that of univariate GPR models. We have found that constructing multivariate GPR models for multiple CC is more efficient than constructing separate univariate GPR models as the multivariate GPR models are able to quantify the uncertainty of the CC outputs as they consider the correlation between the different outputs.

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Y. Al- Taweel for the photography and short autobiography, see TWMS J. App. and Eng. Math. V.12, N.1.