Summer 6-26-2019

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Abstract: As for the robust parameter design of functional responses, a Bayesian Seemingly Unrelated Regression (SUR) model is proposed to take into account the model uncertainty and response variability in this paper. First of all, the SUR model is used to build the functional relationship between the output responses and the input factors at different time points. Also, Bayesian analysis of the SUR model is performed to consider the influence of the model parameter uncertainty on the research results. Secondly, the process means and variances of the functional responses at different time points are estimated by the posterior samples of the simulated responses. Moreover, an integrated performance index (i.e. mean square error) is establish by using the above process means and variances. Then, the optimal parameter settings may be found by minimizing the MSE performance index. Finally, the advantages of the proposed method are illustrated by an example from the literature.
Key Words: Robust parameter design, functional responses, Bayesian analysis, Seemingly Unrelated Regression

1. INTRODUCTION

With the rapid development of digital manufacturing and the increasing complexity of production processes, the quality characteristics of products or processes usually take on a specific functional relationship in the manufacturing process of some complex products. Such kind of functional relationships may be more adequate to describe the quality characteristics of a product or process[1]. This output response is the curve of observed variable called *functional responses*[2], that is to say, the output response is a curve function of the observed variable in one experiment, which can be either controllable or uncontrollable, and the shape or profile of the curve observed at different observed variables determines the quality characteristics of the output response[3]. As for traditional multi-response robust parameter design, the robust parameter design goal of the functional responses is to find the optimal value of the controllable factor, so that the output response is robust and the system is not sensitive to changes in the noise factor. Fogliatto[4] converts the functional response to a normal response based on the Hausdorff distance (HD), the result of which is given by a single value. HD measures the distance between points in the two contours, allowing us to use the distance of the targeted contour as an optimization criterion. In contrast to Euclidean distance calculations, the use of HD does not require input data vectors to have the same dimensions. Furthermore, there is no need to model functional results with HD. Govaerts[5] analyzed possible methods for designing experimental results when the response was functional and compared it to case studies in the metal injection molding industry, proposing three different approaches to fit the model to functional data: two-step nonlinear modeling; pointwise functional regression; and smoothed functional regression. All derived models are capable of predicting functional responses from any design factor level selected in the experimental domain. Castillo[6] proposed a Bayesian modeling method for functional response systems to optimize the shape or profile of functional responses. In the case of a hypothetical robust parameter design scheme where there are controllable factors and noise factors that vary randomly according to a specific distribution, this method introduced the model parameter uncertainty into the optimization phase and extended Peterson's early

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methods to functional responses based on hierarchical two-order mixed-effects models. Wu[7] has some similarities with the work proposed by Castillo, both of which optimize the contour shape with controllable factors and noise factors. The main difference between the two is that the model proposed by Wu, all design parameters are controllable, and the additional variance qualitative model in the second level is considered. Each design point of multiple contours is used for model estimation, so Wu's model estimation is more complicate.

However, the robust parameter design of functional response often ignores the correlation between functional responses, resulting in an increase estimation error of model parameter. Shah and Montgomery[8] first introduced the SUR method into the response surface problem of multi-response experiments. The core of the SUR method is to use the structure of the variance-covariance matrix between the equations to improve the accuracy of the least squares estimation of a single equation[9]. Using the SUR method can produce more accurate model parameter estimates than the least squares method, and reduce the model fitting error caused by the correlation between the response variables, but the SUR method has higher requirements on the sample size of the experiment[10]. Zhang[11] solved the problem of the strong correlation between responses by combining principal component analysis with SUR method and reduces model fitting error. Zhang[12] combined the SUR method into the multivariate quality loss function. The model fitting of the least squares method proved that the SUR method can be used to obtain more accurate parameter estimation of multi-response surface equations when the correlation between the responses is significant. And the expected quality loss at the best solution obtained is smaller. In view of the model parameter uncertainty, Long[13] analyzed the nonparametric seemingly unrelated regression model by the Bayesian method in the study of consumption expenditure and income structure. The results show that the proposed method is effective. Peremans[14] considered robust inferences for seemingly unrelated regression models, and developed fast and robust bootstrap procedures to obtain robust inferences for these estimators, established confidence intervals for model parameters, and regressions in seemingly unrelated regression models. Hypothesis testing of linear coefficient constraints proposes a robust process to test for the existence of correlations between multiple variables. Peterson et al.[15] used a multivariate posterior probability distribution of an unrelated regression model to determine the optimal factor level by evaluating the reliability of the desired multivariate response. The SUR model can be modified by considering the noise distribution and the residual t-distribution model. Further research in this field to make the variance-covariance matrix of controllable factors may also be helpful to the experimenter.

The distribution of the output quality characteristics of many functional responses is changing over a given time interval in industrial production. Therefore, the specifications, target value, as well as the process mean, and variance is also changing with time. For example, environmental engineers may be interested on the influence that different filtering devices have on the concentration of water impurities as time progresses. As for the robust parameter design of functional responses, a Bayesian Seemingly Unrelated Regression (SUR) model is proposed to take into account the model uncertainty and response variability in this paper. First of all, the SUR model is used to build the functional relationship between the output responses and the input factors at different time points. Also, Bayesian analysis of the SUR model is performed to consider the influence of the model parameter uncertainty on the research results. Secondly, the process means and variances of the functional responses at different time points are estimated by the posterior samples of the simulated responses. Moreover, an integrated performance index (i.e. weighted mean square error) is establish by using the above process means and variances. Then, the optimal parameter settings may be found by minimizing the WMSE performance index. Finally, the advantages of the proposed method are illustrated by an example from the literature.

2. Bayesian analysis of SUR models

In the robust parameter design of functional responses, if there are q quality characteristics, the SUR regression model of functional responses can be expressed as:

$$\mathbf{y}_i = \mathbf{X}_i\boldsymbol{\beta}_i + \boldsymbol{\varepsilon}_i \qquad i = 1, 2, ..., q$$
$$\mathbf{E}[\boldsymbol{\varepsilon}_i \boldsymbol{\varepsilon}_j'] = \begin{cases} \sigma_{ii}\mathbf{I}_\mathbf{n}, & i = j \\ \sigma_{ij}\mathbf{I}_\mathbf{n}, & i \neq j \end{cases} \tag{1}$$

where $\mathbf{y}_i$ is the column vector of the observation value of the $n \times 1$ dimensional output response, $\mathbf{X}_i$ is the $n \times p_i$ factor matrix, and $\boldsymbol{\beta}_i$ is the $p_i \times 1$ dimensional estimated error column vector, $\boldsymbol{\varepsilon}_i$ is the $n \times 1$ dimensional random error column vector. As shown in equation (1), the equations have different independent variables and variances. Also, the model permits error terms in different equations to be correlated.

In the matrix form, the SUR model in equation (1) is expressed as:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \boldsymbol{\varepsilon} \sim N(0, \ \Sigma \otimes \mathbf{I}_\mathbf{n}) \tag{2}$$

where 0 is the zero matrix, $\otimes$ is the tensor product, Σ is the $q \times q$ matrix with the diagonal elements $\left\{\sigma_1^2, ..., \sigma_q^2\right\}$, and the off-diagonal ij th elements are σ_{ij} .The maximum likelihood estimates of $\boldsymbol{\beta}$ and Σ are obtained from the maximum likelihood function:

$$f(\mathbf{y} \mid \mathbf{X}, \boldsymbol{\beta}, \Sigma) = \frac{1}{(2\pi)^{nq/2} \mid \Sigma \mid^{n/2}} \exp\left[-\frac{1}{2}\mathrm{tr}\left\{R\Sigma^{-1}\right\}\right] \tag{3}$$

where "tr" denotes the trace of a matrix, $|\Sigma| = \det(\Sigma)$ is the value of the determinant of Σ, the ij^{th} elements of the $q \times q$ matrixmatrix $R = (r_{ij})$, $r_{ij} = (\mathbf{y}_i - \mathbf{X}_i\boldsymbol{\beta}_i)^{\mathrm{T}}(\mathbf{y}_i - \mathbf{X}_i\boldsymbol{\beta}_i)$. If Σ is known, a parameter estimate can be obtained as the generalized least squares (GLS) estimator $\hat{\boldsymbol{\beta}}$. In practice, however, Σ in $\hat{\boldsymbol{\beta}}$ is usually unknown. In this paper, the iterative SUR approach is used to obtain the maximum likelihood estimates of $\boldsymbol{\beta}$ and Σ.

In the absence of prior knowledge, Bayesian analysis with noninformative priors is widespread in practice. This paper used Jeffreys' invariant prior[16]:

$$\pi_1(\boldsymbol{\beta}, \Sigma) = \pi_1(\boldsymbol{\beta})\pi_1(\Sigma) \propto |\Sigma|^{-\frac{q+1}{2}} \tag{4}$$

which is proportional to the square root of the determinant of the Fisher information matrix. The joint posterior density function for the parameters is then:

$$\pi_1(\boldsymbol{\beta}, \Sigma \mid \mathbf{y}, \mathbf{X}) \propto |\Sigma|^{-(n+q+1)/2} \exp\left[-\frac{1}{2}\mathrm{tr}\left\{R\Sigma^{-1}\right\}\right] \tag{5}$$

It is evident from the form of the joint posterior density function $\pi_1(\boldsymbol{\beta}, \Sigma \mid \mathbf{y}, \mathbf{X})$ that the conditional posteriors $\pi_1(\boldsymbol{\beta} \mid \mathbf{y}, \mathbf{X}, \Sigma)$ and $\pi_1(\Sigma \mid \mathbf{y}, \mathbf{X}, \boldsymbol{\beta})$ are

$$\pi_1(\boldsymbol{\beta} \mid \mathbf{y}, \mathbf{X}, \Sigma) = N(\hat{\boldsymbol{\beta}}, \hat{\Omega}) \tag{6}$$
$$\pi_1(\Sigma \mid \mathbf{y}, \mathbf{X}, \boldsymbol{\beta}) = IW(R, n) \tag{7}$$

Where, $\hat{\boldsymbol{\beta}} = \left\{\mathbf{X}'(\Sigma^{-1} \otimes \mathbf{I}_n)\mathbf{X}\right\}^{-1} \mathbf{X}'(\Sigma^{-1} \otimes \mathbf{I}_n)\mathbf{y}$, $\hat{\Omega} = \left\{\mathbf{X}'(\Sigma^{-1} \otimes \mathbf{I}_n)\mathbf{X}\right\}^{-1}$, $IW(\cdot,\cdot)$ denotes the inverse Wishart distribution. Although the posteriors of $\boldsymbol{\beta}$ and Σ are depending upon each other, we can use the Gibbs sampler. Starting from an initial value $\boldsymbol{\beta}^{(0)}$ and $\Sigma^{(0)}$, update the coefficient vector $\boldsymbol{\beta}^{(j)}$ by drawing a new value from the conditional posterior density function $\pi_1(\boldsymbol{\beta} \mid \mathbf{y}, \mathbf{X}, \Sigma^{(j-1)})$ in equation (6), and update $\Sigma^{(j)}$ by drawing a new value from the condition posterior density function $\pi_1(\Sigma \mid \mathbf{y}, \mathbf{X}, \boldsymbol{\beta}^{(j)})$ in equation (7). The convergence diagnostics of model parameter is carried out after discarding the Burn-times of **Nsim** repeated samples. Then, the process means and variances of the functional responses at different time points are estimated by the posterior samples of the simulated responses. Moreover, an integrated performance index (i.e. mean square error) is establish by using the above process means and variances. Finally, the optimal parameter settings may be found by minimizing the MSE performance index. The implemented steps of the proposed method are summarized as followed:

Step 1: The functional relationship between the output responses and the input factors at different time points is established using Bayesian SUR model.

Step 2: Convergence diagnostics for model parameters has performed by using some visual tools (trace plots, autocorrelation plots and posterior density plots).

Step 3: The process means and variances of the functional responses at different time points are estimated by using these stable posterior samples of the simulated responses.

Step 4: An integrated performance index (i.e. mean square error MSE) is establish by using the above process means and variances estimated in Step 3.

Step 5: The optimal parameter settings are minimized using the MSE performance index.

3. CASE ANALYSIS

In the pharmaceutical manufacturing industry, researchers often need to observe the time-oriented dynamic quality characteristics of experimental drugs to determine whether the rate of absorption or dissolution of experimental drugs meet the intent of the patient. Usually, the researchers pre-defined acceptable levels of absorption, especially for controlled-release experimental drugs. If the drug dosage is released too quickly, it may be harmful to the patient, whereas if the dissolution time is considerably less than the target time of release, the therapeutic effect of the drug may not be achieved. The case data in this paper is from a specific solubility study conducted by Nagarwal et al.[17] on in situ gel forming formulation. The in situ gel forming formulation presents a novel idea of delivering the drug to the patient in the form of a liquid dosage, but still achieving the duration required for the controlled release drug to achieve efficacy. It is important to control the release rate of the drug in the blood. By changing the concentration of sodium alginate, gellan gum, and metformin, the release rate of the drug can be controlled within a pre-defined specification. In the experiment conducted by Nagarwal et al., the levels of experimental factors are shown in Table 1. The uncoded factor for sodium alginate (x_1) was set to 1.25%, 1.75%, and 2.25%, the uncoded factor for gellan gum (x_2) was set to 0%, 0.25%, and 0.50%, and the uncoded factor for metformin (x_3)was set to 2.5%, 3.75. % and 5.0%. Changing the concentration of sodium alginate , gellan gum, and metformin, and observed the drug release ratios at three different time points (30 min, 210 min, and 480 min)were respectively y_1, y_2 and y_3 . The expected target values of y_1, y_2 and y_3 are respectively 23.5%, 63.5%, and 92.5%. The experimenter selected a full-factor experiment design to conduct a related experiment. The specific experiment data are shown in Table 2.

Table 1. Test factor levels

Factors	Levels		
	-1	0	1
sodium alginate（%）	1.25	1.75	2.25
gellan gum（%）	0	0.25	0.50
metformin（%）	2.5	3.75	5.0

Table 2. Drugs controlled-release experiment data

Run	Coded units			t_1 (30min)		t_2 (210min)		t_3 (480min)	
	x_1	x_2	x_3	y_1	s_1	y_2	s_2	y_3	s_3
1	-1	-1	-1	35.79	0.73	73.78	1.19	98.29	1.46
2	0	-1	-1	27.43	0.96	65.75	0.73	96.57	0.33
3	1	-1	-1	22.80	3.61	70.11	1.24	92.61	0.79
4	-1	0	-1	32.55	2.90	67.24	0.69	94.46	1.24

Run	Coded units			t_1 (30min)		t_2 (210min)		t_3 (480min)	
	x_1	x_2	x_3	y_1	s_1	y_2	s_2	y_3	s_3
5	0	0	-1	26.06	1.45	62.17	0.48	89.81	1.22
6	1	0	-1	23.50	1.19	56.65	0.49	82.09	1.71
7	-1	1	-1	24.70	1.93	71.76	0.95	91.89	1.46
8	0	1	-1	22.14	1.20	67.11	1.19	86.28	1.92
9	1	1	-1	20.94	0.95	51.47	1.93	80.80	0.05
10	-1	-1	0	48.58	0.55	83.26	0.74	98.57	0.76
11	0	-1	0	40.43	0.92	73.87	0.76	97.70	0.40
12	1	-1	0	37.15	0.73	66.75	1.48	94.93	0.40
13	-1	0	0	32.86	0.56	68.47	0.57	95.58	0.53
14	0	0	0	29.97	0.93	64.74	0.91	92.68	0.74
15	1	0	0	28.00	1.10	58.00	0.38	86.34	0.95
16	-1	1	0	29.06	1.11	69.10	1.46	94.12	0.74
17	0	1	0	25.25	0.92	64.05	1.88	93.70	1.16
18	1	1	0	24.32	0.74	54.12	0.92	84.36	0.57
19	-1	-1	1	41.27	1.04	84.64	0.72	99.52	0.73
20	0	-1	1	37.09	0.98	77.12	1.87	94.75	0.95
21	1	-1	1	25.31	0.64	70.61	0.98	91.64	0.87
22	-1	0	1	37.45	3.39	75.00	2.04	97.23	1.58
23	0	0	1	30.82	0.80	70.22	0.61	93.09	0.85
24	1	0	1	22.82	0.99	59.64	0.21	87.54	1.43
25	-1	1	1	35.93	0.70	73.33	0.99	98.12	1.07
26	0	1	1	32.08	0.99	70.91	1.21	94.93	0.65
27	1	1	1	31.52	0.59	60.37	0.80	88.57	0.42

Combined with MCMC (Markov chain Monte Carlo) method, the experiment generated various coefficients by iterating 7000 times, of which the first 1000 iterations (Burn-in terms) are discarded because the initial iteration has dependencies. In view of the limited space, this paper only gives the trace plot, autocorrelation plot and posterior distribution plot of the partial coefficients for the response y_1.

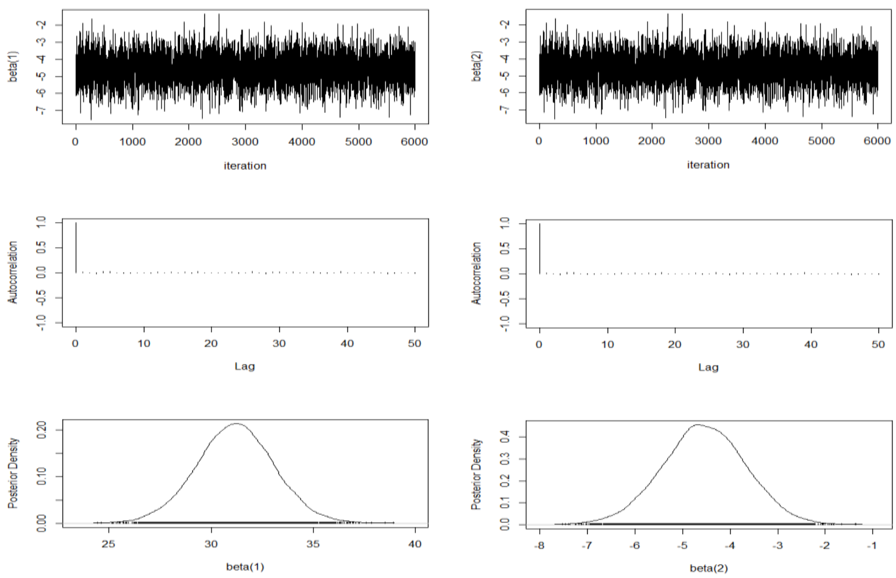

Figure 1. Convergence diagnostics for model parameters

It can be seen from the trace plot in Figure 1 that the generated posterior samples obey the stationary distribution. Also, it can be seen from the autocorrelation plot that the autocorrelation plot of the model parameter is very small, which meets the requirements of convergence diagnosis. The posterior distribution plot of the model parameters showed that the posterior distribution of the coefficients approximates to the normal distribution, which verifies the rationality of the coefficients which follow the normal distribution and ensures the accuracy of the subsequent experimental results.

According to the experimental data in Table 2, the posterior mean of the corresponding regression coefficients can be calculated by the proposed method of this paper. The model is given as follows:

$$y_1(\mathrm{x}) = 31.1730 - 4.5632x_1 - 3.8780x_2 + 3.2565x_3 + 0.6497x_1^2 + 1.8254x_2^2 - 3.3683x_3^2 + 2.3021x_1x_2 - 0.7549x_1x_3 + 1.1756x_2x_3$$

$$\sigma_1^2(\mathrm{x}) = 0.9275 - 1.1317x_1 - 0.0573x_2 - 0.2674x_3 + 0.2822x_1^2 - 0.4082x_2^2 + 0.5459x_3^2 - 0.3467x_1x_2 - 0.2595x_1x_3 + 0.0722x_2x_3$$

$$y_2(\mathrm{x}) = 64.5085 - 6.6081x_1 - 4.6334x_2 + 3.1032x_3 - 0.9949x_1^2 + 4.6181x_2^2 + 1.2846x_3^2 - 1.1808x_1x_2 - 0.6385x_1x_3 - 0.6907x_2x_3$$

$$\sigma_2^2(\mathrm{x}) = 0.7609 - 0.0541x_1 + 0.0920x_2 + 0.0320x_3 - 0.0846x_1^2 + 0.4593x_2^2 + 0.0069x_3^2 - 0.0672x_1x_2 - 0.2132x_1x_3 - 0.1217x_2x_3$$

$$y_3(\mathrm{x}) = 92.4757 - 4.3847x_1 - 2.8745x_2 + 1.8084x_3 - 1.2514x_1^2 + 2.2067x_2^2 - 0.9862x_3^2 - 1.0948x_1x_2 + 0.1681x_1x_3 + 2.0212x_2x_3$$

$$\sigma_3^2(\mathrm{x}) = 0.8970 - 0.1302x_1 + 0.0757x_2 - 0.0898x_3 + 0.0149x_1^2 - 0.3204x_2^2 + 0.3444x_3^2 - 0.1083x_1x_2 + 0.0767x_1x_3 - 0.1042x_2x_3$$

Based on the established model, MSE (mean square error) is selected as the optimization index. The optimization model is given as follows:

$$\min \quad \mathrm{MSE}[y(1), y(2), ..., y(w)] = \sum_{q=1}^{w}[(y(\mathrm{x})\text{-}\mathrm{T(q)})^2 + \sigma^2(\mathrm{x})]$$

Table 3. Experimental results and comparison

Approach	(x_1, x_2, x_3)	MSE[y(1)+y(2)+y(3)]
Nagarwal's methodology	(0,1,0)	91.8266
Goethals's methodology[18]	(-0.1354,0.7544,-0.4700)	14.6293
Proposed methodology	(1,-0.8862,-1)	8.8753

According to the above optimization model, the genetic algorithm is used to optimize the parameters, and the experimental results and comparison are shown in Table 3.

It can be seen from Table 3 that the total mean square error obtained by the proposed method is 8.8753 and the optimal parameter settings are $x_1 = 1, x_2 = -0.8862, x_3 = -1$ respectively when the functional response has different target values at different time points. Compared with the method proposed by Nagarwal, the total mean square error is reduced by 90.33%; Compared with the Goethals's method, and the total mean square error is reduced by 39.33%. The method proposed in this paper and Goethals and Nagarwal are all optimized for the process mean of a given target value at the time point. Compared with the other two methods, the proposed method has been dramatically improved based on the performance index MSE. In addition, the proposed method combines the simultaneous optimization of process mean and variance, thereby reducing the total mean square error observed in the approximate objective function.

4. CONCLUSIONS

The correlation among multiple responses and the model parameter uncertainty are often neglected in the study of the robust parameter design of functional responses. The proposed method in this paper not only takes into account the dynamic characteristics of functional responses over time but also considered the model parameter uncertainty and the correlation between functional responses as well as the robustness of multivariate processes. As for the robust parameter design of functional response based on the response surface method, the accuracy of model estimation is crucial for the reliability of optimization results. It is worth noting that the proposed approach provides a natural way of combining prior information (e.g., experience of experimenters) with experimental data in the laser micro-drilling process. When new experimental data become available, the previous posterior distribution can be used as a prior. Future research can be conducted to continually update the posterior distribution of the SUR models with the experimental data obtained by means of sequential experimental design. By doing so, the proposed approach can build a more reasonable and flexible process model to reflect the high variability and uncertainty of the advanced manufacturing process. In addition, the proposed approach only focuses on the optimal setting of the controllable factors in this paper. However, it also significantly reduces the variation which is transmitted by the noise. Therefore, as to our belief, the current research work can be further extended to achieve online robust parameter design that accounts for uncertainty of noise factors and allows the user to update the model estimates with online observations.

5. ACKNOWLEDGEMENT

This work is supported by the National Natural Science Foundation of China (Nos. 71771121) and the Fundamental Research Funds for the Central Universities (No.3091511102).

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