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A Bayesian Parameter Estimation Approach to Response Surface Optimization in Quality Engineering

Elif Kozan^{*1}, Onur Köksoy²

Abstract

In recent years, Bayesian analyses have become increasingly popular for solving industrial related problems. This paper illustrates the use of Bayesian methods in response surface methodology (RSM) in the context of “off-line quality” improvement. RSM and Bayesian Linear Regression - an approach which uses the prior information to make a more efficient inference - are considered together. Results from different estimators are compared for the first time ever. Bayesian linear regression uses the prior information in the high uncertainty state of the response function to make more efficient and more realistic inferences than can be obtained with classical regression. Several different values of the prior distribution of the parameter and uncertainty analysis will be presented for comparative purposes. The effect of the change in the prior information and variances will be illustrated by using an example from the literature.

Keywords: Response surface methodology, Bayesian regression, off-line quality control, experimental design, WinBUGS

1. INTRODUCTION

In general, the Bayesian approach is a special form of Bayes’ theorem, which was first introduced by Thomas Bayes [1]. Subsequently Laplace [16] presented the general form of Bayes’ theorem. In the 20th century, Laplace’s studies have received considerable attention from authors such as Keynes [11], Ramsey [21], and Savage [22]. Jeffreys [10] made some important contributions to the fundamental theory of Bayesian statistics. Metropolis et al. [17] introduced the Metropolis-Hastings algorithm. Along with new technologies in computer sciences, this algorithm has been used to overcome the computational difficulties connected with integrals of problems involving Bayesian models. Hasting [8] introduced the Monte Carlo method for evaluating integrals as a

major tool for practical Bayesian inference. In addition, the development of techniques such as Markov chain Monte Carlo (MCMC) has greatly increased the applicability of the Bayesian approach. Goldstein [6] applied the Bayesian approach to regression problems.

The development of fast computers made necessary calculations faster and pioneered the use of the Bayesian approach for a wide range of applications. Also, a review of the literature reveals that the estimation step becomes more powerful and more realistic when using prior model information. In Bayesian inference, the Bayes’ risk function includes both a posterior model of unknown parameters given the observation and a cost of error function. By minimizing this risk function, one easily obtains the point estimators

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using Bayesian methodology. A couple of different methods are available for Bayesian estimation, including maximum a posteriori (MAP), minimum mean square error (MMSE), and Markov chain Monte Carlo algorithms.

By utilizing Bayesian philosophy with a focus on quality purposes in RSM, it seems more realistic results might be obtained by comparison with the results of classical regression. Taguchi [12,25] presented a robust design method based on statistical experimental design and quality engineering concepts. This method, along with Taguchi's philosophy, received a great deal of attention, but it seemed to have some statistical shortcomings. Box [2] has criticized Taguchi's method and revealed its shortcomings. Based on his criticism, RSM, first presented by Box and Wilson [3], was popularized in the early 1990s as a tool for improving the quality. Vining and Myers [13,14,15,27] proposed an alternative off-line quality improvement approach (i.e., dual response approach) by combining RSM and the good properties of Taguchi's method. This novel approach to RSM has become popular and is widely quoted in the literature.

There are some studies available related to the Bayesian approach for estimates of response surface model parameters. Steinberg[23] presented a Bayesian approach to empirical regression modeling in which the response function was represented by a power series expansion in Hermite polynomials. Chen[4] used Bayesian hierarchical regression modelling approach to dual response surface. Moreover, Bayesian analysis provides inference about the uncertainty of the model parameters. Chen and Ye[5] applied the Bayesian hierarchical model on dual response surface to partially replicated designs and the performance of the Bayesian model was compared with least squares methods by using simulated data under various mean and variance models. Peterson et al.[20] presented a Bayesian predictive approach to multiresponse optimization experiments. Quesada et al. [24] presented a Bayesian approach and consist of maximizing the posterior predictive probability that the process satisfies a set of constraints on the responses. Türkşen's study [26] was analyzed of response

surface model parameters, which was obtained by using Bayesian approach and fuzzy approach, through interval analysis.

This study aims to apply Bayesian estimation methods to RSM with a focus area of quality improvement. The research will consider various Bayesian estimates and investigate their effects of using a prior model on the mean and variance responses. Different estimators generate different solutions depending on the influence of the selected prior information.

The rest of this paper is organized as follows: In the following section a brief overview of selected Bayesian estimation methods is presented. An estimation process of common regression coefficients of data modeling, linked to a discussed Bayesian estimation method, is put forward in Section 3. The next section illustrates the findings and offers a brief discussion of experimental design, including Bayesian analyses to RSM. Finally, the paper ends with a conclusion.

2. BAYESIAN PARAMETER ESTIMATION

In terms of the Bayesian approach, point estimation of a parameter vector θ is usually the mean of the posterior distribution based on minimization of the following Bayesian conditional risk function:

$$R(\hat{\theta}|\mathbf{y}) = \int_{\theta} C(\hat{\theta}, \theta) f(\theta|\mathbf{y}) d\theta \quad (2.1)$$

where $C(\hat{\theta}, \theta)$ is the cost function and $f(\theta|\mathbf{y})$ is the posterior density of θ , given an observation vector \mathbf{y} . More methods to find Bayesian estimators will be presented. The reader is referred to Vaseghi (2000) for details.

2.1. Maximum a posteriori estimation (MAP)

The MAP method is based on maximization of the posterior distribution. According to this method, the cost function is assumed to be uniformly distributed, defined as,

$$C(\hat{\theta}, \theta) = 1 - \delta(\hat{\theta}, \theta) \quad (2.2)$$

where $\delta(\hat{\theta}, \theta)$ is the Kronecker delta function. Then, the conditional risk function is given by,

$$R(\hat{\theta}|\mathbf{y})_{MAP} = \int_{\theta} (1 - \delta(\hat{\theta}, \theta))f(\theta|\mathbf{y})d\theta \quad (2.3)$$

By using equation (2.3), when the posterior function $f(\theta|\mathbf{y})$ attains a maximum, the minimum Bayesian risk can be achieved (see Figure 2.1 in [28]). Hence, the MAP estimator is given in equation (2.4). Here, the MAP estimator is the mode of the posterior distribution.

$$\hat{\theta}_{MAP} = \operatorname{argmax}_{\theta} f(\theta|\mathbf{y}) = \operatorname{argmax}_{\theta} [f(\mathbf{y}|\theta) f(\theta)] \quad (2.4)$$

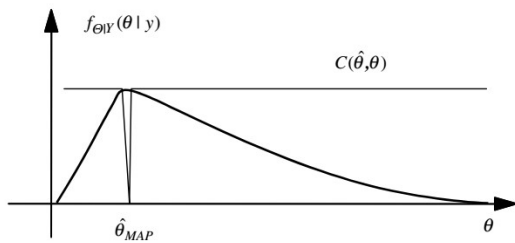


Figure 2.1 The Bayesian cost function for the MAP estimate

2.2. Minimum mean square error estimation (MMSE)

The MMSE method minimizes the mean square error cost function. The conditional risk function is

$$R(\hat{\theta}|\mathbf{y})_{MMSE} = E((\hat{\theta} - \theta)^2|\mathbf{y}) = \int_{\theta} (\hat{\theta} - \theta)^2 f(\theta|\mathbf{y})d\theta \quad (2.5)$$

By minimizing equation (2.5) with respect to parameter θ , the MMSE estimator is obtained as

$$\hat{\theta}_{MMSE} = \int_{\theta} \theta f(\theta|\mathbf{y})d\theta \quad (2.6)$$

Figure 2.2, taken from [28], illustrates the mean square error cost function and the Bayesian estimate:

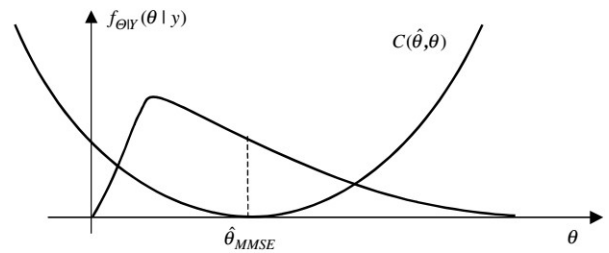


Figure 2.2 Bayesian cost function graph for the MMSE estimate

2.3. Estimation of parameters using MCMC by WinBUGS

As the third estimation strategy, the posterior distribution is obtained by the MCMC method in WinBUGS, which was created in the 1990s as a free software package. WinBUGS uses Gibbs sampling as a special case of the Metropolis-Hastings algorithm.

Let $f(\theta_j | \theta_{\setminus j}, \mathbf{y})$ be the full conditional posterior distribution, where θ is the parameter vector such as $\theta_{\setminus j} = (\theta_1, \dots, \theta_{j-1}, \theta_{j+1}, \dots, \theta_d)^T$ and $\mathbf{y} = (y_1, y_2, \dots, y_n)^T$ be the vector of length n of the response data. For a particular state of the chain $\theta^{(t)}$, the new parameter values have been obtained by Gibbs sampling as follows [19]:

$$\begin{aligned} \theta_1^{(t)} &\sim f(\theta_1 | \theta_2^{(t-1)}, \theta_3^{(t-1)}, \dots, \theta_p^{(t-1)}, \mathbf{y}), \\ \theta_2^{(t)} &\sim f(\theta_2 | \theta_1^{(t)}, \theta_3^{(t-1)}, \dots, \theta_p^{(t-1)}, \mathbf{y}), \\ \theta_3^{(t)} &\sim f(\theta_3 | \theta_1^{(t)}, \theta_2^{(t)}, \dots, \theta_p^{(t-1)}, \mathbf{y}), \\ \theta_p^{(t)} &\sim f(\theta_p | \theta_1^{(t)}, \theta_2^{(t)}, \dots, \theta_{p-1}^{(t)}, \mathbf{y}) \end{aligned}$$

After these generations, the Monte Carlo error might be observable. This error represents the standard error of the estimation made by the Markov chain algorithm. Therefore the iteration continues until this error becomes less than 0.05 (e.g., as small as possible).

3. BAYESIAN ESTIMATION OF REGRESSION MODELS

Bayesian estimation and data modeling constitute a useful method, as it can be used in a wide range of areas, including signal processing, computer vision processes, genome data analysis, and industrial applications.

Regression modeling defines the functional relationship between a dependent random variable and another set of independent variables. Let $\mathbf{y} = (y_1, \dots, y_n)^T$ be the n -dimensional column vector, and let \mathbf{X} be the $n \times p$ matrix whose i^{th} row is x_i . Then the classical regression assumption is

$$\{\mathbf{y}|\mathbf{X}, \boldsymbol{\beta}, \sigma^2\} \sim \text{multivariate normal}(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I}) \tag{3.1}$$

where \mathbf{I} and σ^2 are the $p \times p$ identity matrix and variance of the model, respectively. The sampling density of the data, as a function of parameter vector $\boldsymbol{\beta}$, is

$$p\{\mathbf{y}|\mathbf{X}, \boldsymbol{\beta}, \sigma^2\} \propto e^{\{-\frac{1}{2\sigma^2}[\mathbf{y}^T\mathbf{y} - 2\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{y} + \boldsymbol{\beta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}]\}} \tag{3.2}$$

if $\boldsymbol{\beta} \sim \text{multivariate normal}(\boldsymbol{\beta}_0 = \boldsymbol{\beta}_{\text{prior}}, \boldsymbol{\Sigma}_0 = \boldsymbol{\Sigma}_{\text{prior}})$, then

$$p(\boldsymbol{\beta}|\mathbf{y}, \mathbf{X}, \sigma^2) \propto p(\mathbf{y}|\boldsymbol{\beta}, \mathbf{X}, \sigma^2)p(\boldsymbol{\beta}) = e^{\{\boldsymbol{\beta}^T(\boldsymbol{\Sigma}_0^{-1}\boldsymbol{\beta}_0 + \frac{\mathbf{X}^T\mathbf{y}}{\sigma^2}) - \frac{1}{2}\boldsymbol{\beta}^T(\boldsymbol{\Sigma}_0^{-1} + \frac{\mathbf{X}^T\mathbf{X}}{\sigma^2})\boldsymbol{\beta}\}} \tag{3.3}$$

This result seemed to be proportional to a multivariate normal density, with

$$\boldsymbol{\Sigma}_{MMSE}^* = \text{var}(\boldsymbol{\beta}|\mathbf{y}, \mathbf{X}, \sigma^2) = (\boldsymbol{\Sigma}_0^{-1} + \frac{\mathbf{X}^T\mathbf{X}}{\sigma^2})^{-1} \tag{3.4}$$

and

$$\boldsymbol{\beta}_{MMSE}^* = E(\boldsymbol{\beta}|\mathbf{y}, \mathbf{X}, \sigma^2) = (\boldsymbol{\Sigma}_0^{-1} + \frac{\mathbf{X}^T\mathbf{X}}{\sigma^2})^{-1}(\boldsymbol{\Sigma}_0^{-1}\boldsymbol{\beta}_0 + \mathbf{X}^T\mathbf{y}/\sigma^2) \tag{3.5}$$

$$= \boldsymbol{\Sigma}_{MMSE}^* \left(\boldsymbol{\Sigma}_{\text{prior}}^{-1}\boldsymbol{\beta}_{\text{prior}} + \left(\frac{\mathbf{X}^T\mathbf{X}}{\sigma^2}\right)\boldsymbol{\beta}_{\text{classical}} \right)$$

If the elements of the prior precision matrix $\boldsymbol{\Sigma}_0^{-1}$ are small, then the conditional expectation

$E(\boldsymbol{\beta}|\mathbf{y}, \mathbf{X}, \sigma^2)$ is approximately equal to the least squares estimate (known as MMSE). Also, the MAP estimators are defined as follows (see [9]):

$$\boldsymbol{\beta}_{MAP}^* = (\boldsymbol{\Sigma}_{\text{prior}}^{-1}\sigma^2 + \mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}_{\text{classical}} + (\boldsymbol{\Sigma}_{\text{prior}}^{-1}\sigma^2 + \mathbf{X}^T\mathbf{X})^{-1}\sigma^2\boldsymbol{\Sigma}_{\text{prior}}^{-1}\boldsymbol{\beta}_{\text{prior}} \tag{3.6}$$

and the variance-covariance matrix is

$$\boldsymbol{\Sigma}_{MAP}^* = (\boldsymbol{\Sigma}_{\text{prior}}^{-1}\sigma^2 + \mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\sigma^2((\boldsymbol{\Sigma}_{\text{prior}}^{-1}\sigma^2 + \mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T)^T. \tag{3.7}$$

4. BAYESIAN APPROACH TO RESPONSE OPTIMIZATION

Let us consider the experiment discussed in [7],[18]. The study involves three factors, namely $X_1, X_2,$ and X_3 . The goal is to find the combination of factor levels that maximizes the amount (in grams) of crystal growth. Table 4.1 presents the experimental data.

When RSM applies to the experimental setup, the second order estimated response surface is

$$\hat{Y}_{\text{classical}} = 97.58 + 1.36X_2 - 1.49X_3 - 12.06X_2^2 - 9.23X_3^2 \tag{4.1}$$

According to this model, the optimum response is found at $\hat{Y}_{\text{max}} = 97.68$ grams, which is illustrated in Figure 4.1 when the coded variables are $x_2 = 0.05646$ and $x_3 = -0.08097$.

Table 4.1 A central composite design of three variables

Run	x_1	x_2	x_3	y	Run	x_1	x_2	x_3	y
1	-1	-1	-1	66	11	0	-1.682	0	68
2	-1	-1	1	70	12	0	1.682	0	63
3	-1	1	-1	78	13	0	0	-1.682	65
4	-1	1	1	60	14	0	0	1.682	82
5	1	-1	-1	80	15	0	0	0	113
6	1	-1	1	70	16	0	0	0	100
7	1	1	-1	100	17	0	0	0	118
8	1	1	1	75	18	0	0	0	88
9	-1.682	0	0	100	19	0	0	0	100
10	1.682	0	0	80	20	0	0	0	85

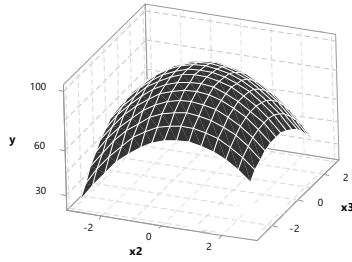


Figure 4.1 Response surface graph of maximum growth

4.1 Bayesian MMSE estimator approach to response optimization

Let the unknown β parameter for the prior distribution of the model be $\beta \sim \text{Normal}(\beta_{\text{prior}}, \Sigma_{\text{prior}})$. Consider different prior means and variances on the parameters. For example the parameters β have a multivariate normal prior distribution as used by Gilmour and Mead [7] with mean $\beta_{\text{prior}} = [100, 0, 0, -6, -6]$ and diagonal variance matrix with each element on the diagonal being 10. For illustration $\sigma^2 = 1$ was assumed [7]. Another assumption for mean $\beta_{\text{prior}} = [110, 0, 0, -6, -6]$ and diagonal variance matrix with each element on the diagonal being 1 also $\sigma^2 = 158,7$ was assumed. These assumptions were used in combination with each other. Also, the classical coefficient vector from the classical regression is given as $\beta_{\text{classical}}$. In Bayesian MMSE, the expected value model of the posterior distribution can be found by using equation (3.5), as follows:

$$\beta_{\text{MMSE}}^* = \begin{bmatrix} 97.56355 \\ 1.35119 \\ -1.48318 \\ -12.02238 \\ -9.21221 \end{bmatrix}$$

and using equation (3.4),

$$\Sigma_{\text{MMSE}}^* = \begin{bmatrix} 0.11793 & 0 & 0 & -0.05016 & -0.05016 \\ 0 & 0.07268 & 0 & 0 & 0 \\ 0 & 0 & 0.07268 & 0 & 0 \\ -0.05016 & 0 & 0 & 0.06795 & 0.00587 \\ -0.05016 & 0 & 0 & 0.00587 & 0.06795 \end{bmatrix}$$

Using these results, the optimum response is found to be $\hat{Y}_{\text{max}} = 97.66$ grams when the coded variables are $x_2 = 0.05619$, and $x_3 = -0.08050$.

However, if one uses the classical regression estimator $\sigma^2 = 158.7$ rather than $\sigma^2 = 1$ in the MMSE estimation process, the optimum response becomes $\hat{Y}_{\text{max}} = 97.48$ with $x_2 = 0.03221$, and $x_3 = -0.04136$.

4.2 Bayesian MAP estimator approach to response optimization

Second, consider the MAP estimator. For instance, the prior information is chosen as $\beta'_{\text{prior}} = [110, 0, 0, -6, -6]$ and the classical variance estimator is $\sigma^2 = 158.7$. The other assumptions mentioned in the previous section are applied for this estimator and the results are given in the final summary Table 4.3. In Bayesian MAP, by using the given prior information, the expected value model of the posterior distribution can be found by using equation (3.6), as follows:

$$\beta_{\text{MAP}}^* = \begin{bmatrix} 108.12898 \\ 0.10830 \\ -0.11888 \\ -7.66978 \\ -7.40964 \end{bmatrix} \quad \text{and using equation (3.7),}$$

$$\Sigma_{\text{MAP}}^* = \begin{bmatrix} 0.08364 & 0 & 0 & 0.04764 & 0.04764 \\ 0 & 0.07324 & 0 & 0 & 0 \\ 0 & 0 & 0.07324 & 0 & 0 \\ -0.04764 & 0 & 0 & 0.10452 & 0.02099 \\ -0.04764 & 0 & 0 & 0.02099 & 0.10452 \end{bmatrix}$$

Using these results, the optimum response is found as $\hat{Y}_{\text{max}} = 108.13$ grams when the coded variables are $x_2 = 0.00706$, and $x_3 = -0.00802$.

4.3 Using MCMC by WinBUGS approach to response optimization

Finally, by using WinBUGS for the in prior informations. For instance $\beta_{\text{prior}} = [110, 0, 0, -6, -6]$ and $\sigma^2 = 158.7$; the WinBUGS output is presented in Table 4.2. The other assumptions mentioned in section 4.1 are applied for this problem and the results are given in the final summary Table 4.3. Examining the model parameters in the output, the autocorrelation is a way of measuring the independence of the simulated values. According to Figure 4.2, no autocorrelation exists for the model parameters.

Table 4.2 Posterior summaries of the regression parameters

node	mean	sd	MC error	2.5%	median	97.5%	start	sample
beta0	103.1	2.361	0.04592	98.61	103.1	107.8	1001	3000
beta1	0.6199	2.253	0.04154	-3.947	0.6127	4.911	1001	3000
beta2	-0.648	2.286	0.0346	-5.151	-0.6756	3.956	1001	3000
beta3	-11.35	2.137	0.04135	-15.56	-11.33	-7.145	1001	3000
beta4	-10.03	2.161	0.04004	-14.21	-10.05	-5.741	1001	3000

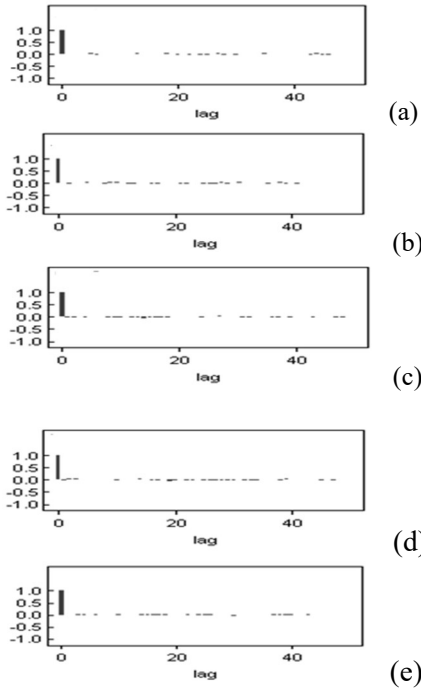


Figure 4.2 Plots for the autocorrelation functions of the chains: (a) β_0 , (b) β_1 , (c) β_2 , (d) β_3 , (e) β_4

Using these Bayesian regression coefficients obtained by WinBUGS, the optimum response is found as $\hat{Y}_{max} = 103.12$ grams when the coded variables are $x_2 = 0.02731$, and $x_3 = -0.03230$.

The output in Figure 4.3 gives a trace of the actual values of the chain and information about simulation convergences. It seems the Markov chain quickly converges to the final distribution. Also, according to the Kernel density plots with 3000 sample sizes in Figure 4.4, one realizes that the posterior distributions of the parameters are close to the normal density.

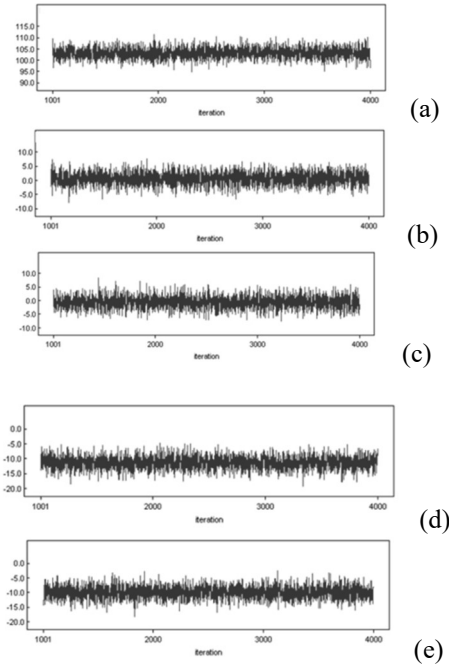


Figure 4.3 Convergence plots for the parameter chains: (a) β_0 , (b) β_1 , (c) β_2 , (d) β_3 , (e) β_4

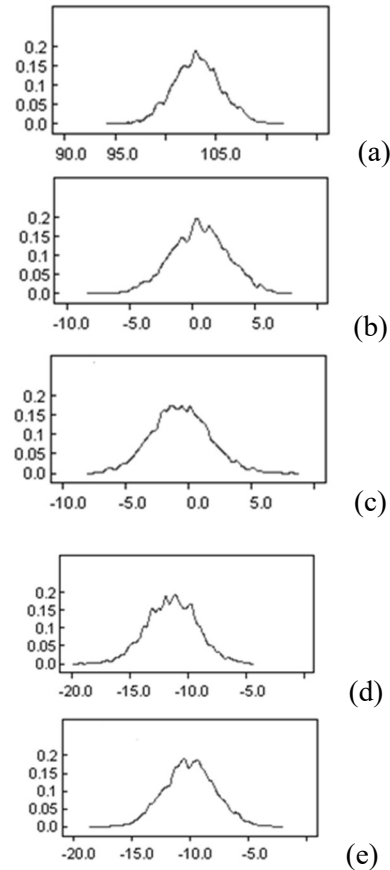


Figure 4.4 Plots for the posterior pdfs of the parameter chains: (a) β_0 , (b) β_1 , (c) β_2 , (d) β_3 , (e) β_4

4.4. Final summary

The summary results about the mean and the variance of posterior distributions and the optimum response values based on different prior information are given in Table 4.3

Table 4.3. Optimum response values for different prior information and different variance

Prior Expectation	Prior Variance Σ_{prior} (diagonal)	Variance	Bayesian Regression with RSM			
			Response (MMSE)	Response(MA P)	Response (WinBUGS)	
$\beta_{prior} = [100, 0, 0, -6, -6]$	1	$\sigma^2 = 158.7$	99.16	99.16	99.14	
	10		97.48	97.48	97.5	
$\beta_{prior} = [110, 0, 0, -6, -6]$	1		108.14	108.14	108.1	
	10		103.10	103.13	103.12	
$\beta_{prior} = [100, 0, 0, -6, -6]$	1		$\sigma^2 = 1$	97.52	97.52	97.52
	10			97.66	97.66	97.66
$\beta_{prior} = [110, 0, 0, -6, -6]$	1	98.55		98.55	98.54	
	10	97.78		97.78	97.78	

5. CONCLUSION

In this article, the application of Bayesian methods to RSM is studied. Bayesian regression estimators are obtained by using various priors and two different variance assumptions (see Table 4.3). These estimators are utilized as Bayesian regression estimators and their posterior information is revealed. Then, RSM is applied to such posterior information and a comparison is made between these emerging results and the results obtained by classical RSM.

According to the comparison results, where the situations of the prior variance (Σ_{prior} diagonal) are smaller, then the estimated Bayesian responses are generally bigger than the classical responses. However, the higher prior expected value (β_{prior}) assigns, the higher estimated Bayesian responses compared with the classical method. In other words, the prior information must be chosen carefully, otherwise this leads to

different solutions rather than the one obtained by the classical response surface method.

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