

Analysing Four Factor Second Order Models Using Response Surface Methodology with Application in Germination of *Melia volkensii*

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Abstract

*Second order models are useful in situations where there are curvilinear effects present in the true response function. Such models have real life applications in a wide variety of fields such as agriculture, biology, and business among others. In such cases the problem is twofold. First is to fit a model for the relationship between the dependent variable and the explanatory variables. Second is to find the values of the predictor variables that optimize the response. The objectives here were to fit second order models involving four independent variables as well as to obtain values for the explanatory variables that optimize the dependent variable. Response surface methodology (RSM) is used both to fit the models as well as to analyze the fitted surfaces. The data obtained by simulation were from a four factor rotatable central composite design (CCD). Results included the fitted models and the tests of adequacy of fit for the models. Optimal values for the independent variables were also given. Contour and surface plots are presented to give a pictorial view of the nature of the response surface. As an application a model for the germination of *Melia volkensii* experiment was fitted and optimal values of temperature, soil pH and chemical concentration obtained. The work in this paper can be directly applied in many instances where an investigator studies the relationship between four predictor variables and a response. With some relevant adjustments this can be extended to any number of explanatory variables.*

Keywords: Response surface methodology, Second order model, Optimal; Four factors an Central composite design.

INTRODUCTION

Response surface methodology (RSM) is a collection of mathematical and statistical techniques that is useful for the modelling and analysis of problems in which a response of interest is influenced by several variables and the objective is to optimize this response (Montgomery, 2005).

The RSM was initially developed and described by Box and Wilson, (1951). Hill and Hunter, (1966) conducted an extensive review of the literature for RSM emphasizing especially on the practical applications of the method. Mead and Pike, (1975) examined the state of RSM from the statistician's point of view and investigated the extent to which the methodology is used in applied research with particular emphasis on biometric applications. Myers, Khuri and Carter, (1989) evaluated the use of RSM between 1966 and 1988. Over the years RSM has been applied in a wide variety of fields. Examples of the recent applications include (Madamba, 2002), (Hussain *et al.*, 2011), (Pishgar-Komleh *et al.*, 2012), (Anwar *et al.*, 2012), (Hussain and Uddin, 2012), (Krishnaa *et al.*, 2013) and (Zainal *et al.*, 2013)

This paper focuses on the analysis of four factor second order models using RSM. In section 2 second order models are discussed and some of its applications on real life problems. Section 3 concentrates on the procedures of analysing four factor second order models using RSM. Some simulation results and experimental results are presented in section 4. Finally, in Section 5 some conclusions and recommendations are made on the use of four factor second order models.

Second Order Models

The general approach of the response surface methodology is to use first order models to move to the optimum region and then higher order models to explore this region. When the first order model is found to be inadequate, a second degree model should be fitted and appropriate analysis performed on the fitted model.

The second order response surface is of the form:

$$y = \beta_0 + \sum_{i=1}^p \beta_i x_i + \sum_{i=1}^p \beta_{ii} x_i^2 + \sum_{i < j} \beta_{ij} x_i x_j + \varepsilon \quad (1)$$

For p=4, the model becomes

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{44} x_4^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{14} x_1 x_4 + \beta_{23} x_2 x_3 + \beta_{24} x_2 x_4 + \beta_{34} x_3 x_4 + \varepsilon \quad (2)$$

There are several designs that are used for second order response models. Examples include the 3^k designs, the Box-Behken design and the central composite design developed by (Box and Wilson, 1951). In this paper, the central composite design to study second order models were used.

Analysis of Four Factor Second Order Models

When the experimenter is relatively close to the optimum, the second order model is an adequate approximation.

The second order fitted model is of the form

$$\hat{y} = b_0 + \sum_{i=1}^p b_i x_i + \sum_{i=1}^p B_{ii} x_i^2 + \sum_{i < j} \sum B_{ij} x_i x_j \quad (3)$$

In matrix notation this is

$$\hat{y} = b_0 + x' \hat{\mathbf{b}} + x' \hat{\mathbf{B}} x \quad (4)$$

Where b_0 , $\hat{\mathbf{b}}$ and $\hat{\mathbf{B}}$ are estimates of the intercept, linear and second order coefficients respectively. $x' = (x_1, x_2, \dots, x_p)$, $\hat{\mathbf{b}}' = (b_1, b_2, \dots, b_p)$ and $\hat{\mathbf{B}}$ is the $p * p$ symmetric matrix

$$\hat{\mathbf{B}} = \begin{bmatrix} b_{11} & \frac{b_{12}}{2} & \dots & \frac{b_{1p}}{2} \\ \frac{b_{12}}{2} & b_{22} & \dots & \frac{b_{2p}}{2} \\ & & \ddots & \\ \frac{b_{1p}}{2} & & & b_{pp} \end{bmatrix} \quad (5)$$

Location of the Stationary Point

The stationary point is the one in which the response has an optimum value (maximum or minimum)

From differential calculus, this point is obtained differentiating the dependent variable and equating to zero to obtain the corresponding values of the independent variable. In this case,

$$\hat{y} = b_0 + x' \hat{\mathbf{b}} + x' \hat{\mathbf{B}} x \quad (6)$$

$$\frac{\partial \hat{y}}{\partial x} = \hat{\mathbf{b}} + 2 \hat{\mathbf{B}} x \quad (7)$$

Setting the derivative equal to 0, one can solve for the stationary point of the system:

$$x_s = -\frac{1}{2} \hat{\mathbf{B}}^{-1} \hat{\mathbf{b}} \quad (8)$$

The predicted response at the stationary point is:

$$\hat{y}_s = b_0 + \frac{1}{2} x_s' \hat{\mathbf{b}} \quad (9)$$

Canonical Analysis

There are several ways to examine the fitted second order response surface. Initially it is desirable to plot response contours. This is done by setting \hat{y} to some specified value y_0 and tracing out contours relating x_1, x_2, \dots, x_p .

An alternative procedure is to reduce the equation to its canonical form. That is done by forming the equation:

$$\hat{y} = \hat{y}_s + \sum_{i=1}^p \lambda_i w_i^2 \quad (10)$$

where \hat{y}_s , the estimated stationary point is the center of the contours and w_i 's are a new set of axes called the principal axes. The coefficients λ_i 's are the eigenvalues of \hat{B} and give the shape of the surface such that:

If $\lambda_1, \lambda_2, \dots, \lambda_p$ are all negative, the stationary point is a point of maximum response.

If $\lambda_1, \lambda_2, \dots, \lambda_p$ are all positive, the stationary point is a point of minimum response.

If $\lambda_1, \lambda_2, \dots, \lambda_p$ are mixed in sign, the stationary point is a saddle point.

The relative sizes of the eigenvalues also tell a great deal. For example, if most of the eigenvalues are large positive numbers but a few are near zero, then there is a ridge in the graph of the response function. Moving along that ridge will make little difference in the value of the response but might make a big difference in some other aspect of the system, like cost, for example.

The w_i 's are obtained as follows: For a matrix M with columns equal to the normalized eigenvectors of \hat{B} , then $M' \hat{B} M = \Lambda$ where Λ is a diagonal matrix with diagonal elements equal to the eigenvalues of \hat{B} .

Let

$$z = x - x_s, w = M'z. \text{ Now, } \hat{y} = b_0 + x' \hat{b} + x' \hat{B} x$$

$$\hat{y} = b_0 + (z + x_s)' \hat{b} + (z + x_s)' \hat{B} (z + x_s) \quad (11)$$

$$\hat{y} = b_0 + z' \hat{b} + x_s' \hat{b} + (z' \hat{B} + x_s' \hat{B})(z + x_s) \quad (12)$$

$$\hat{y} = b_0 + z' \hat{b} + x_s' \hat{b} + z' \hat{B} z + x_s' \hat{B} z + z' \hat{B} x_s + x_s' \hat{B} x_s \quad (13)$$

$$\hat{y} = [b_0 + x_s' \hat{b} + x_s' \hat{B} x_s] + z' \hat{b} + z' \hat{B} z + 2x_s' \hat{B} z \quad (14)$$

But $x_s = -\frac{1}{2} \hat{B}^{-1} \hat{b}$. This implies $2x_s' \hat{B} z = -z' \hat{B} \hat{B}^{-1} \hat{b} = -z' \hat{b}$. Therefore:

$$\hat{y} = \hat{y}_s + z' \hat{B} z \quad (15)$$

Changing the coordinate system:

$$\hat{y} = \hat{y}_s + w' M' \hat{B} M w \quad (16)$$

$$\hat{y} = \hat{y}_s + w' \Lambda w \quad (17)$$

For $p = 4$,

$$\hat{y} = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3 + b_4 x_4 + B_{11} x_1^2 + B_{12} x_1 x_2 + B_{13} x_1 x_3 + B_{14} x_1 x_4 + B_{22} x_2^2 + B_{23} x_2 x_3 + B_{24} x_2 x_4 + B_{33} x_3^2 + B_{34} x_3 x_4 + B_{44} x_4^2 \quad (18)$$

Its canonical form equivalent is:

$$\hat{y} = \hat{y}_s + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \lambda_3 w_3^2 + \lambda_4 w_4^2 \tag{19}$$

where $\lambda_1, \lambda_2, \lambda_3$ and λ_4 are the eigenvalues of

$$\hat{B} = \begin{bmatrix} B_{11} & \frac{B_{12}}{2} & \frac{B_{13}}{2} & \frac{B_{14}}{2} \\ \frac{B_{12}}{2} & B_{22} & \frac{B_{23}}{2} & \frac{B_{24}}{2} \\ \frac{B_{13}}{2} & \frac{B_{32}}{2} & B_{33} & \frac{B_{34}}{2} \\ \frac{B_{14}}{2} & \frac{B_{24}}{2} & \frac{B_{34}}{2} & B_{44} \end{bmatrix} \tag{20}$$

$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} m_{11} & m_{21} & m_{31} & m_{41} \\ m_{12} & m_{22} & m_{32} & m_{42} \\ m_{13} & m_{23} & m_{33} & m_{43} \\ m_{14} & m_{24} & m_{34} & m_{44} \end{bmatrix} \begin{bmatrix} x_1 - x_{1s} \\ x_2 - x_{2s} \\ x_3 - x_{3s} \\ x_4 - x_{4s} \end{bmatrix} \tag{21}$$

$\begin{bmatrix} m_{11} & m_{21} & m_{31} & m_{41} \\ m_{12} & m_{22} & m_{32} & m_{42} \\ m_{13} & m_{23} & m_{33} & m_{43} \\ m_{14} & m_{24} & m_{34} & m_{44} \end{bmatrix}'$ being a matrix with columns equal to the normalized eigenvectors of \hat{B} .

Empirical Study

Description of the Empirical Study

Data were simulated corresponding to the three possible response surfaces; maximum response, minimum response and saddle response. There were three replicates for each of these cases. The design was a rotatable four factor central composite design. The models used in the simulation were:

Maximum response

$$y = 10 + 0.8x_1 + 0.5x_2 + 0.3x_3 + 0.1x_4 - 2x_1^2 - 1.7x_1x_2 + 1.4x_1x_3 + 1.2x_1x_4 - 1.6x_2^2 + 0.9x_2x_3 + 0.4x_2x_4 - 0.8x_3^2 - 0.5x_3x_4 - 0.6x_4^2 + \varepsilon \tag{22}$$

Minimum response

$$y = 10 + 0.8x_1 - 0.5x_2 + 0.3x_3 + 0.1x_4 + 2x_1^2 - 1.7x_1x_2 + 1.4x_1x_3 - 1.2x_1x_4 + 1.6x_2^2 - 0.9x_2x_3 + 0.4x_2x_4 + 0.8x_3^2 - 0.5x_3x_4 + 0.6x_4^2 + \varepsilon \tag{23}$$

Saddle response

$$y = 10 + 0.8x_1 + 0.5x_2 + 0.3x_3 - 0.1x_4 - 2x_1^2 + 1.7x_1x_2 + 1.4x_1x_3 + 1.2x_1x_4 + 1.6x_2^2 - 0.9x_2x_3 + 0.4x_2x_4 + 0.8x_3^2 + 0.5x_3x_4 - 0.6x_4^2 + \varepsilon \tag{24}$$

For each of the models $\varepsilon \sim N(0,1)$

The simulated data are given below

Table 1: Simulated Data for the Maximum, Minimum and Saddle Response Models

Design Variables				Maximum			Minimum			Saddle		
x_1	x_2	x_3	x_4	y_1	y_2	y_3	y_1	y_2	y_3	y_1	y_2	y_3
-1	-1	-1	-1	4	4	4	11	11	10	11	12	12
1	-1	-1	-1	5	5	4	18	18	19	7	7	8
-1	1	-1	-1	8	9	9	15	16	18	11	10	10
1	1	-1	-1	0	1	3	13	11	11	11	10	11
-1	-1	1	-1	2	2	4	14	15	14	10	11	11
1	-1	1	-1	7	7	9	20	20	18	10	10	12
-1	1	1	-1	8	7	5	12	10	9	6	7	7
1	1	1	-1	5	5	5	19	18	16	13	14	12
-1	-1	-1	1	3	3	4	13	12	12	9	10	11
1	-1	-1	1	8	8	7	15	15	15	6	6	8
-1	1	-1	1	7	6	5	18	18	18	8	8	6
1	1	-1	1	5	6	4	14	16	16	13	13	14
-1	-1	1	1	0	2	0	14	13	13	9	9	10
1	-1	1	1	10	11	10	18	16	15	12	12	13
-1	1	1	1	4	2	2	15	17	17	5	5	7
1	1	1	1	8	6	4	12	14	12	16	15	15
-2	0	0	0	1	1	0	17	17	18	3	4	5
2	0	0	0	3	3	2	18	20	20	4	3	3
0	-2	0	0	2	1	1	17	17	17	16	15	13
0	2	0	0	5	4	4	16	16	16	19	20	21
0	0	-2	0	7	7	6	9	8	7	14	13	12
0	0	2	0	7	7	6	13	12	12	14	14	14
0	0	0	-2	8	7	9	12	12	12	8	8	9
0	0	0	2	7	9	9	12	11	14	8	9	9
0	0	0	0	11	11	11	9	7	7	10	10	11
0	0	0	0	9	9	8	10	8	9	9	8	9
0	0	0	0	12	13	15	10	9	8	11	11	11
0	0	0	0	9	9	10	9	10	11	12	12	14
0	0	0	0	11	11	13	9	10	11	9	9	9
0	0	0	0	10	9	8	10	9	7	10	10	11

RESULTS AND DISCUSSION

Analysis of the Maximum Response Model

The characteristics of the fitted maximum response models are summarized in tables 2 and 3 below.

Table 2: The Fitted Maximum Response Model

	Replicate I				Replicate II				Replicate III			
	Coeff.	Std. Error	t value	p value	Coeff.	Std. Error	t value	p value	Coeff.	Std. Error	t value	p value
Intercept	10.333	0.390	26.517	0.000	10.333	0.529	19.541	0.000	10.833	0.751	14.427	0.000
x_1	0.667	0.195	3.422	0.004	0.750	0.264	2.837	0.013	0.708	0.375	1.887	0.079
x_2	0.500	0.195	2.566	0.021	0.250	0.264	0.946	0.359	0.042	0.375	0.111	0.913
x_3	0.167	0.195	0.855	0.406	0.000	0.264	0.000	1.000	-0.042	0.375	-0.111	0.913
x_4	0.167	0.195	0.855	0.406	0.333	0.264	1.261	0.227	-0.292	0.375	-0.777	0.449
x_1^2	-2.042	0.182	-11.202	0.000	-2.021	0.247	-8.171	0.000	-2.406	0.351	-6.851	0.000
x_1x_2	-1.875	0.239	-7.857	0.000	-1.625	0.324	-5.018	0.000	-1.438	0.460	-3.126	0.007
x_1x_3	1.250	0.239	5.238	0.000	1.125	0.324	3.474	0.003	1.313	0.460	2.854	0.012
x_1x_4	1.375	0.239	5.762	0.000	1.375	0.324	4.246	0.001	0.938	0.460	2.039	0.060
x_2^2	-1.667	0.182	-9.145	0.000	-1.896	0.247	-7.665	0.000	-2.031	0.351	-5.784	0.000
x_2x_3	0.375	0.239	1.572	0.137	-0.250	0.324	-0.772	0.452	-0.563	0.460	-1.223	0.240
x_2x_4	0.000	0.239	0.000	1.000	-0.500	0.324	-1.544	0.143	-0.438	0.460	-0.951	0.356
x_3^2	-0.792	0.182	-4.344	0.001	-0.771	0.247	-3.117	0.007	-1.156	0.351	-3.292	0.005
x_3x_4	-0.375	0.239	-1.572	0.137	-0.250	0.324	-0.772	0.452	-0.438	0.460	-0.951	0.356
x_4^2	-0.667	0.182	-3.658	0.002	-0.521	0.247	-2.106	0.052	-0.406	0.351	-1.157	0.265
Multiple R^2	0.9571				0.9233				0.8734			
Adjusted R^2	0.9171				0.8517				0.7553			
F statistic	23.9200				12.9000				7.3940			
P value	0.0000				0.0000				0.0002			

Table 2 and table 3 show that all the three models are significant with p values of 0.0000, 0.0000 and 0.0002

Table 3: Analysis of Variance Table for the Maximum Response Model

	Source	Sum of Squares	Degrees of Freedom	Mean Square	F value	P value
Replicate I	Model	305.133	14	21.795	23.920	0.000
	First Order	18.000	4	4.500	4.939	0.010
	Two way interaction	116.000	6	19.333	21.220	0.000
	Pure Quadratic	171.133	4	42.783	46.957	0.000
	Residuals	13.667	15	0.911		
	Lack of fit	6.333	10	0.633	0.432	0.879
	Pure error	7.333	5	1.467		
	Total	318.800	29			
Replicate II	Model	303.000	14	21.643	12.898	0.000
	First Order	17.667	4	4.417	2.633	0.076
	Two way interaction	98.750	6	16.458	9.810	0.000
	Pure Quadratic	186.583	4	46.646	27.802	0.000
	Residuals	25.167	15	1.678		
	Lack of fit	11.833	10	1.183	0.444	0.872
	Pure error	13.333	5	2.667		
	Total	328.167	29			
Replicate III	Model	350.217	14	25.016	7.394	0.000
	First Order	14.167	4	3.542	1.047	0.416
	Two way interaction	85.875	6	14.312	4.230	0.011
	Pure Quadratic	250.175	4	62.544	18.486	0.000
	Residuals	50.750	15	3.383		
	Lack of fit	11.917	10	1.192	0.153	0.994
	Pure error	38.833	5	7.767		
	Total	400.967	29			

The stationary points, eigen values and canonical equivalent models are depicted in table 4 below:

Table 4: Stationary points and Eigenvalues and for the Maximum Response Model

	Stationary Points				Eigenvalues			
	x_1	x_2	x_3	x_4				
Replicate I	0.485	-0.084	0.343	0.529	-0.237	-0.574	-1.238	-3.119
Replicate II	4.629	-3.051	2.697	7.247	-0.028	-0.582	-1.701	-2.898
Replicate III	0.139	-0.028	0.114	-0.245	-0.216	-0.674	-2.036	-3.075

Since for all the replicates all the eigenvalues are negative the response surface is a maximum one.

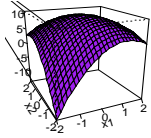
The canonical equivalent forms of the fitted models are respectively for the three replicates;

$$\hat{y} = 10.546 - 0.237w_1^2 - 0.574w_2^2 - 1.238w_3^2 - 3.119w_4^2 \quad (25)$$

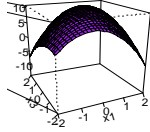
$$\hat{y} = 12.894 - 0.028w_1^2 - 0.582w_2^2 - 1.701w_3^2 - 2.898w_4^2 \quad (26)$$

$$\hat{y} = 10.915 - 0.216w_1^2 - 0.674w_2^2 - 2.036w_3^2 - 3.075w_4^2 \quad (27)$$

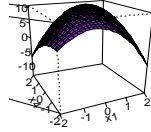
The nature of these responses can be seen in the response surface plots shown in figure 1 and figure 2 below.



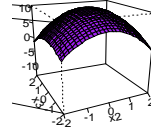
Slice at $x_3 = 0, x_4 = 0$



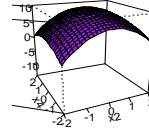
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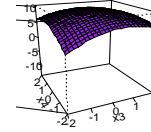
Slice at $x_2 = 0, x_3 = 0$



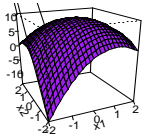
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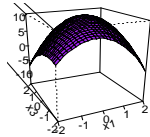
Slice at $x_1 = 0, x_3 = 0$



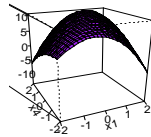
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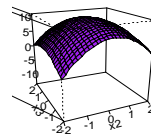
Slice at $x_3 = 0, x_4 = 0$



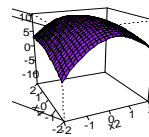
Slice at $x_2 = 0, x_4 = 0$



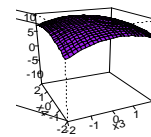
Slice at $x_2 = 0, x_3 = 0$



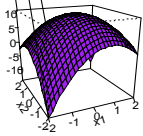
Slice at $x_1 = 0, x_4 = 0$



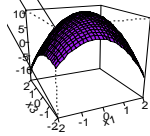
Slice at $x_1 = 0, x_3 = 0$



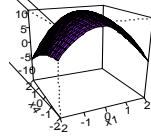
Slice at $x_1 = 0, x_2 = 0$



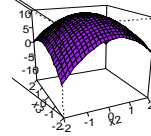
Slice at $x_3 = 0, x_4 = 0$



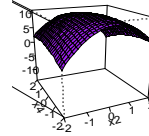
Slice at $x_2 = 0, x_4 = 0$



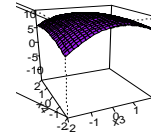
Slice at $x_2 = 0, x_3 = 0$



Slice at $x_1 = 0, x_4 = 0$



Slice at $x_1 = 0, x_3 = 0$



Slice at $x_1 = 0, x_2 = 0$

Figure 1: Response Surface Plot for the Maximum Response Model

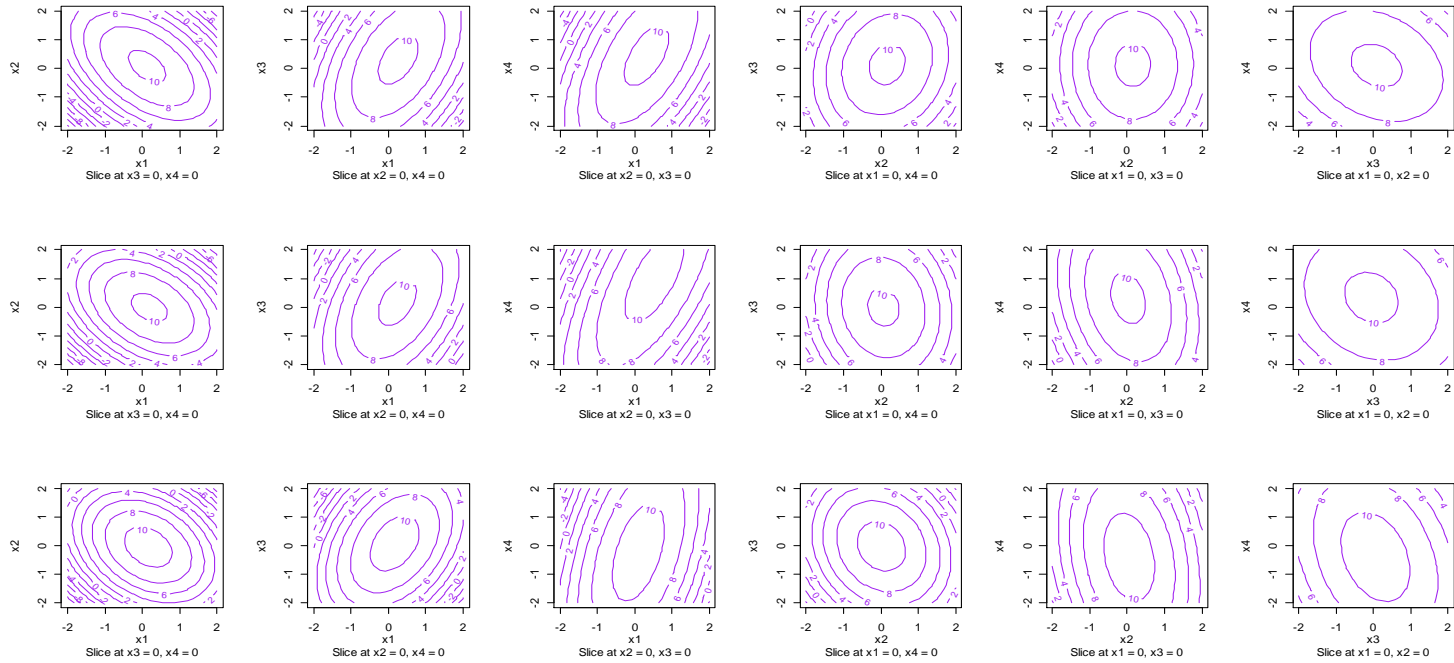


Figure 2: Contour Plot for the Maximum Response Model

Analysis of the Minimum Response Model

The characteristics of the fitted minimum response models are summarized in tables 5 and 6.

The tables show that all the three models are significant with p values of 0.0000, 0.0002 and 0.0040.

Table 5: The Fitted Minimum Response Model

	Replicate I				Replicate II				Replicate III			
	Coeff.	Std. Error	t value	p value	Coeff.	Std. Error	t value	p value	Coeff.	Std. Error	t value	p value
Intercept	9.500	0.570	16.664	0.000	8.833	0.760	11.630	0.000	8.833	0.986	8.963	0.000
x_1	0.792	0.285	2.777	0.014	0.917	0.380	2.414	0.029	0.625	0.493	1.268	0.224
x_2	-0.292	0.285	-1.023	0.322	-0.083	0.380	-0.219	0.829	-0.042	0.493	-0.085	0.934
x_3	0.625	0.285	2.193	0.045	0.583	0.380	1.536	0.145	0.208	0.493	0.423	0.678
x_4	-0.125	0.285	-0.439	0.667	0.000	0.380	0.000	1.000	0.292	0.493	0.592	0.563
x_1^2	2.135	0.267	8.009	0.000	2.563	0.355	7.214	0.000	2.552	0.461	5.537	0.000
x_1x_2	-1.313	0.349	-3.760	0.002	-1.250	0.465	-2.688	0.017	-1.563	0.604	-2.589	0.021
x_1x_3	0.688	0.349	1.969	0.068	0.625	0.465	1.344	0.199	0.313	0.604	0.518	0.612
x_1x_4	-1.188	0.349	-3.402	0.004	-0.875	0.465	-1.881	0.079	-0.938	0.604	-1.553	0.141
x_2^2	1.885	0.267	7.071	0.000	2.063	0.355	5.806	0.000	1.927	0.461	4.181	0.001
x_2x_3	-0.688	0.349	-1.969	0.068	-0.625	0.465	-1.344	0.199	-0.813	0.604	-1.346	0.198
x_2x_4	0.188	0.349	0.537	0.599	1.125	0.465	2.419	0.029	0.938	0.604	1.553	0.141
x_3^2	0.510	0.267	1.914	0.075	0.438	0.355	1.232	0.237	0.177	0.461	0.384	0.706
x_3x_4	-0.563	0.349	-1.611	0.128	-0.500	0.465	-1.075	0.299	-0.188	0.604	-0.311	0.760
x_4^2	0.760	0.267	2.852	0.012	0.813	0.355	2.287	0.037	1.052	0.461	2.282	0.037
Multiple R^2	0.9097				0.8756				0.8010			
Adjusted R^2	0.8254				0.7596				0.6152			
F statistic	10.7900				7.544				4.312			
P value	0.0000				0.0002				0.0040			

Table 6: Analysis of Variance Table for the Minimum Response Model

Source	Sum of Squares	Degrees of Freedom	Mean Square	F value	P value
Replicate I					
Model	294.616	14	21.044	10.792	0.000
First Order	26.833	4	6.708	3.440	0.035
Two way interaction	70.875	6	11.812	6.058	0.002
Pure Quadratic	196.908	4	49.227	25.245	0.000
Residuals	29.250	15	1.950		
Lack of fit	27.750	10	2.775	9.250	0.012
Pure error	1.500	5	0.300		
Total	323.866	29			
Replicate II					
Model	365.550	14	26.111	7.544	0.000
First Order	28.500	4	7.125	2.059	0.137
Two way interaction	74.000	6	12.333	3.563	0.021
Pure Quadratic	263.050	4	65.762	19.000	0.000
Residuals	51.917	15	3.461		
Lack of fit	45.083	10	4.508	3.299	0.100
Pure error	6.833	5	1.367		
Total	417.467	29			
Replicate III					
Model	351.783	14	25.127	4.311	0.004
First Order	12.500	4	3.125	0.536	0.711
Two way interaction	79.875	6	13.312	2.284	0.091
Pure Quadratic	259.408	4	64.852	11.128	0.000
Residuals	87.417	15	5.828		
Lack of fit	70.583	10	7.058	2.097	0.214
Pure error	16.833	5	3.367		
Total	439.200	29			

The stationary points and eigenvalues are depicted in table 7:

Table 7: Stationary points and Eigenvalues for the Minimum Response Model

	Stationary Points				Eigenvalues			
	x_1	x_2	x_3	x_4				
Replicate I	-0.190	-0.107	-0.735	-0.325	2.932	1.447	0.632	0.281
Replicate II	-0.148	-0.067	-0.762	-0.268	3.267	1.685	0.615	0.308
Replicate III	-0.166	-0.238	-1.095	-0.204	3.317	1.464	0.840	0.087

Since for all the replicates all the eigenvalues were positive the response surface is a minimum one.

The canonical equivalent forms of the fitted models are respectively for the three replicates;

$$\hat{y} = 9.231 + 2.932w_1^2 + 1.447w_2^2 + 0.632w_3^2 + 0.281w_4^2 \quad (28)$$

$$\hat{y} = 8.046 + 3.267w_1^2 + 1.685w_2^2 + 0.615w_3^2 + 0.308w_4^2 \quad (29)$$

$$\hat{y} = 8.143 + 3.317w_1^2 + 1.464w_2^2 + 0.840w_3^2 + 0.087w_4^2 \quad (30)$$

The nature of these responses can be seen in the response surface plots shown in figure 3 and figure 4 below.

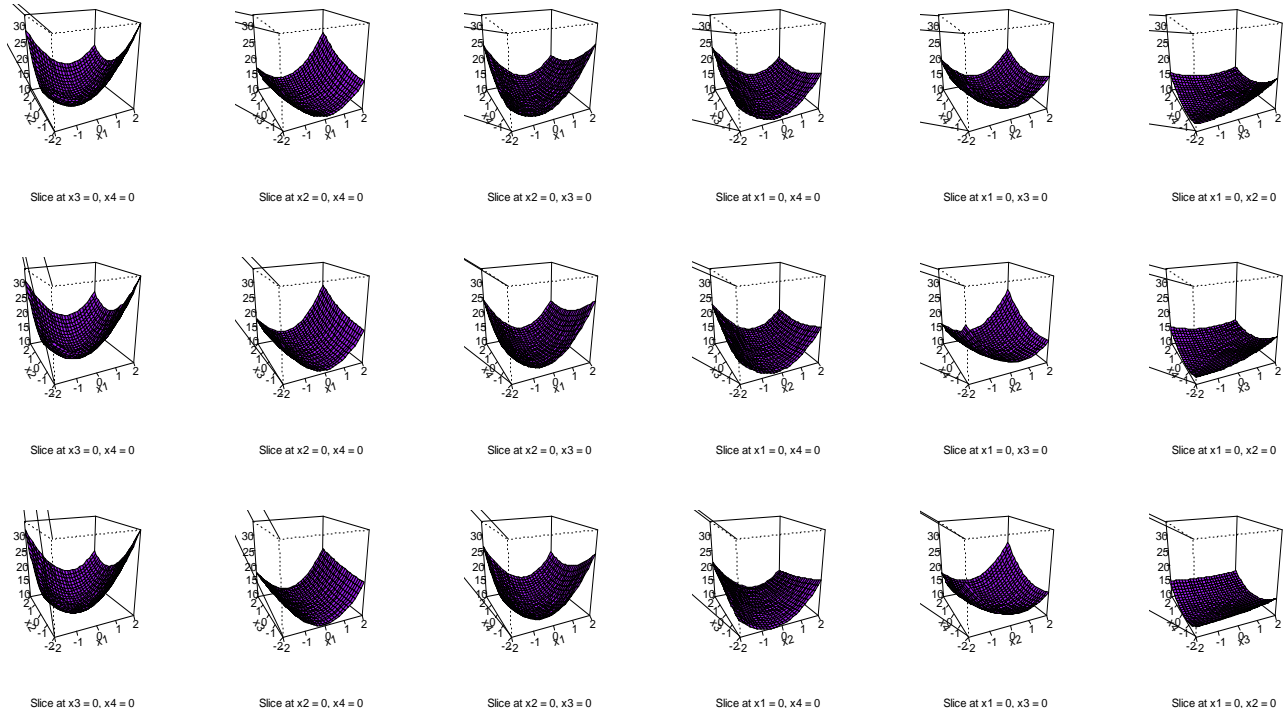


Figure 3: Response Surface Plot for the Minimum Response Model

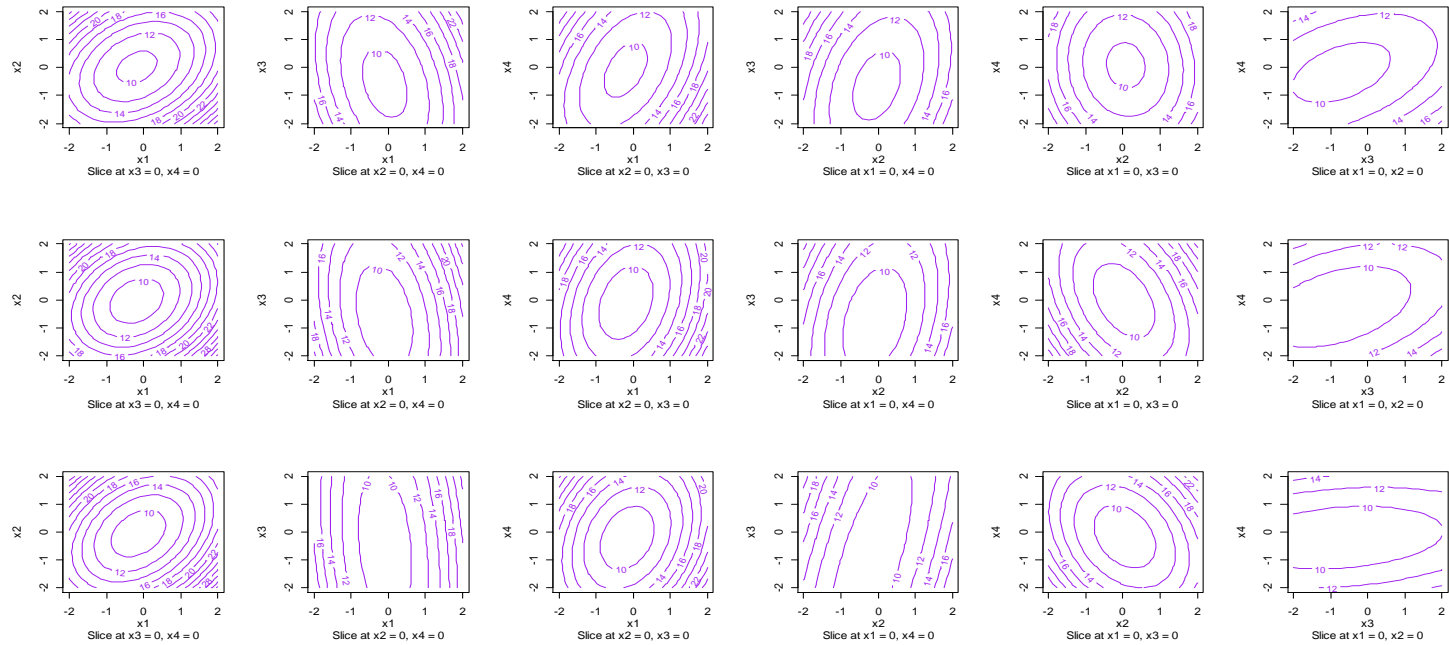


Figure 4: Contour Plot for the Minimum Response Model

Analysis of the Saddle Response Model

The characteristics of the fitted saddle response models are summarized in tables 8 and 9.

The tables show that all the three models were significant with p values of 0.0000, 0.0000 and 0.0035 for the three replicates

Table 8: The Fitted Saddle Response Model

	Replicate I				Replicate II				Replicate III			
	Coeff.	Std. Error	t value	p value	Coeff.	Std. Error	t value	p value	Coeff.	Std. Error	t value	p value
Intercept	10.167	0.468	21.703	0.000	10.000	0.585	17.108	0.000	10.833	0.862	12.564	0.000
x_1	0.875	0.234	3.736	0.002	0.542	0.292	1.853	0.084	0.625	0.431	1.450	0.168
x_2	0.625	0.234	2.668	0.018	0.625	0.292	2.139	0.049	0.542	0.431	1.256	0.228
x_3	0.208	0.234	0.890	0.388	0.375	0.292	1.283	0.219	0.458	0.431	1.063	0.305
x_4	-0.042	0.234	-0.178	0.861	-0.042	0.292	-0.143	0.889	0.042	0.431	0.097	0.924
x_1^2	-1.823	0.219	-8.320	0.000	-1.760	0.273	-6.439	0.000	-1.760	0.403	-4.365	0.001
x_1x_2	1.688	0.287	5.883	0.000	1.813	0.358	5.064	0.000	1.563	0.528	2.959	0.010
x_1x_3	1.438	0.287	5.011	0.000	1.438	0.358	4.016	0.001	0.938	0.528	1.776	0.096
x_1x_4	0.813	0.287	2.832	0.013	0.813	0.358	2.270	0.038	0.813	0.528	1.539	0.145
x_2^2	1.677	0.219	7.655	0.000	1.740	0.273	6.363	0.000	1.490	0.403	3.694	0.002
x_2x_3	-0.688	0.287	-2.397	0.030	-0.438	0.358	-1.222	0.240	-0.438	0.528	-0.829	0.420
x_2x_4	0.188	0.287	0.654	0.523	0.188	0.358	0.524	0.608	0.188	0.528	0.355	0.727
x_3^2	0.802	0.219	3.661	0.002	0.740	0.273	2.705	0.016	0.490	0.403	1.214	0.244
x_3x_4	0.438	0.287	1.525	0.148	0.063	0.358	0.175	0.864	0.313	0.528	0.592	0.563
x_4^2	-0.698	0.219	-3.185	0.006	-0.510	0.273	-1.867	0.082	-0.510	0.403	-1.266	0.225
Multiple R^2	0.9482				0.9174				0.8030			
Adjusted R^2	0.8999				0.8403				0.6230			
F statistic	19.620				11.900				4.424			
P value	0.0000				0.0000				0.0035			

Table 9: Analysis of Variance Table for the Saddle Response Model

	Source	Sum of Squares	Degrees of Freedom	Mean Square	F value	P value
Replicate I	Model	361.716	14	25.837	19.618	0.000
	First Order	28.833	4	7.208	5.475	0.006
	Two way interaction	100.375	6	16.729	12.706	0.000
	Pure Quadratic	232.508	4	58.127	44.147	0.000
	Residuals	19.750	15	1.317		
	Lack of fit	12.917	10	1.292	0.945	0.563
	Pure error	6.833	5	1.367		
	Total	381.466	29			
Replicate II	Model	341.416	14	24.387	11.896	0.000
	First Order	19.833	4	4.958	2.419	0.094
	Two way interaction	99.875	6	16.646	8.120	0.000
	Pure Quadratic	221.708	4	55.427	27.038	0.000
	Residuals	30.750	15	2.050		
	Lack of fit	20.750	10	2.075	1.038	0.517
	Pure error	10.000	5	2.000		
	Total	372.166	29			
Replicate III	Model	276.283	14	19.735	4.424	0.004
	First Order	21.500	4	5.375	1.205	0.349
	Two way interaction	68.875	6	11.479	2.573	0.064
	Pure Quadratic	185.908	4	46.477	10.418	0.000
	Residuals	66.917	15	4.461		
	Lack of fit	50.083	10	5.008	1.488	0.346
	Pure error	16.833	5	3.367		
	Total	343.200	29			

The stationary points, eigenvalues and canonical equivalent models are depicted in table 10:

Table 10: Stationary points and Eigenvalues

	Stationary Points				Eigenvalues			
	x_1	x_2	x_3	x_4				
Replicate I	0.020	-0.234	-0.216	-0.117	1.909	1.035	-0.708	-2.277
Replicate II	-0.062	-0.170	-0.238	-0.136	1.976	0.943	-0.464	-2.246
Replicate III	-0.068	-0.198	-0.433	-0.182	1.690	0.633	-0.503	-2.112

Since for all the replicates the eigenvalues were of mixed sign, the response surface was a saddle one.

The canonical equivalent forms of the fitted models were respectively for the three replicates;

$$\hat{y} = 10.083 + 1.909w_1^2 + 1.035w_2^2 - 0.708w_3^2 - 2.277w_4^2 \quad (31)$$

$$\hat{y} = 9.888 + 1.976w_1^2 + 0.943w_2^2 - 0.464w_3^2 - 2.246w_4^2 \quad (32)$$

$$\hat{y} = 10.655 + 1.690w_1^2 + 0.633w_2^2 - 0.503w_3^2 - 2.112w_4^2 \quad (33)$$

The nature of these responses can be seen in the response surface plots shown in figure 5 and figure 6.

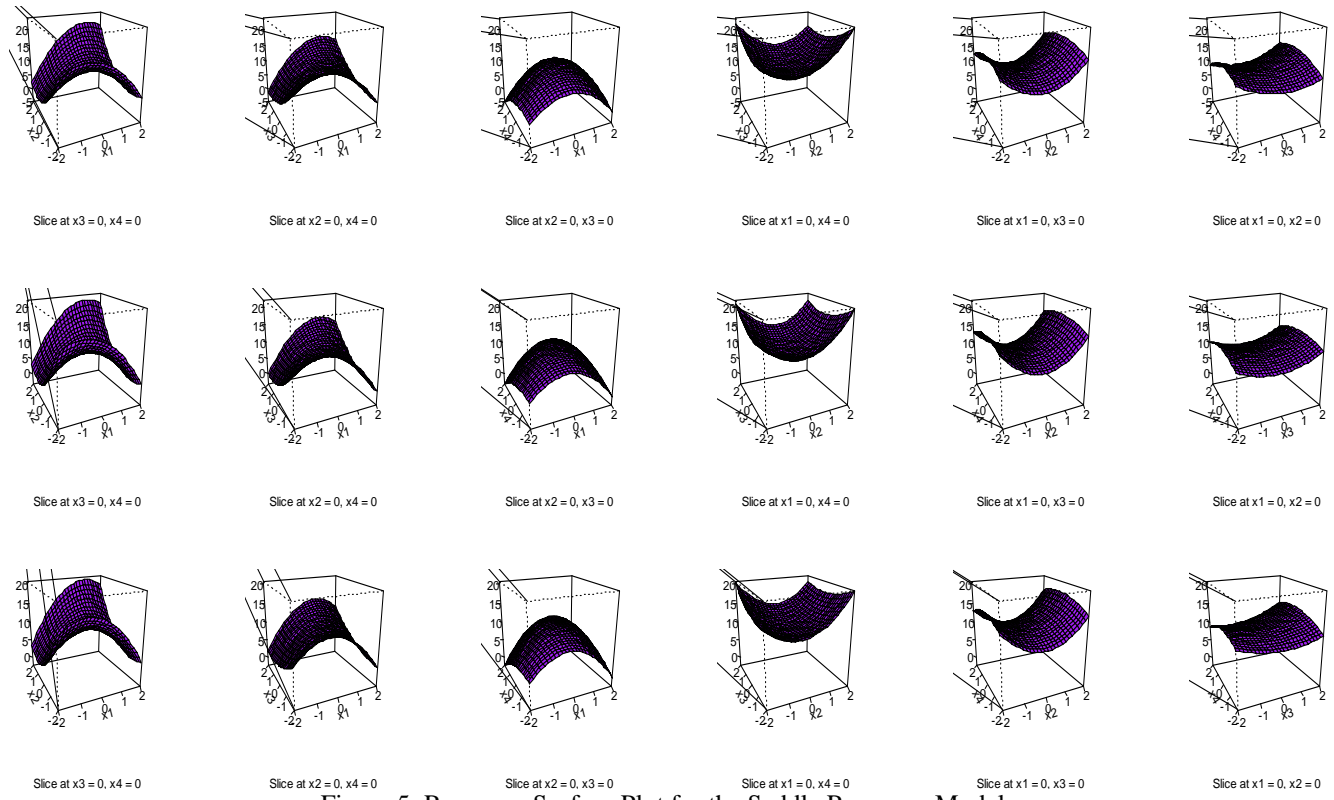


Figure 5: Response Surface Plot for the Saddle Response Model

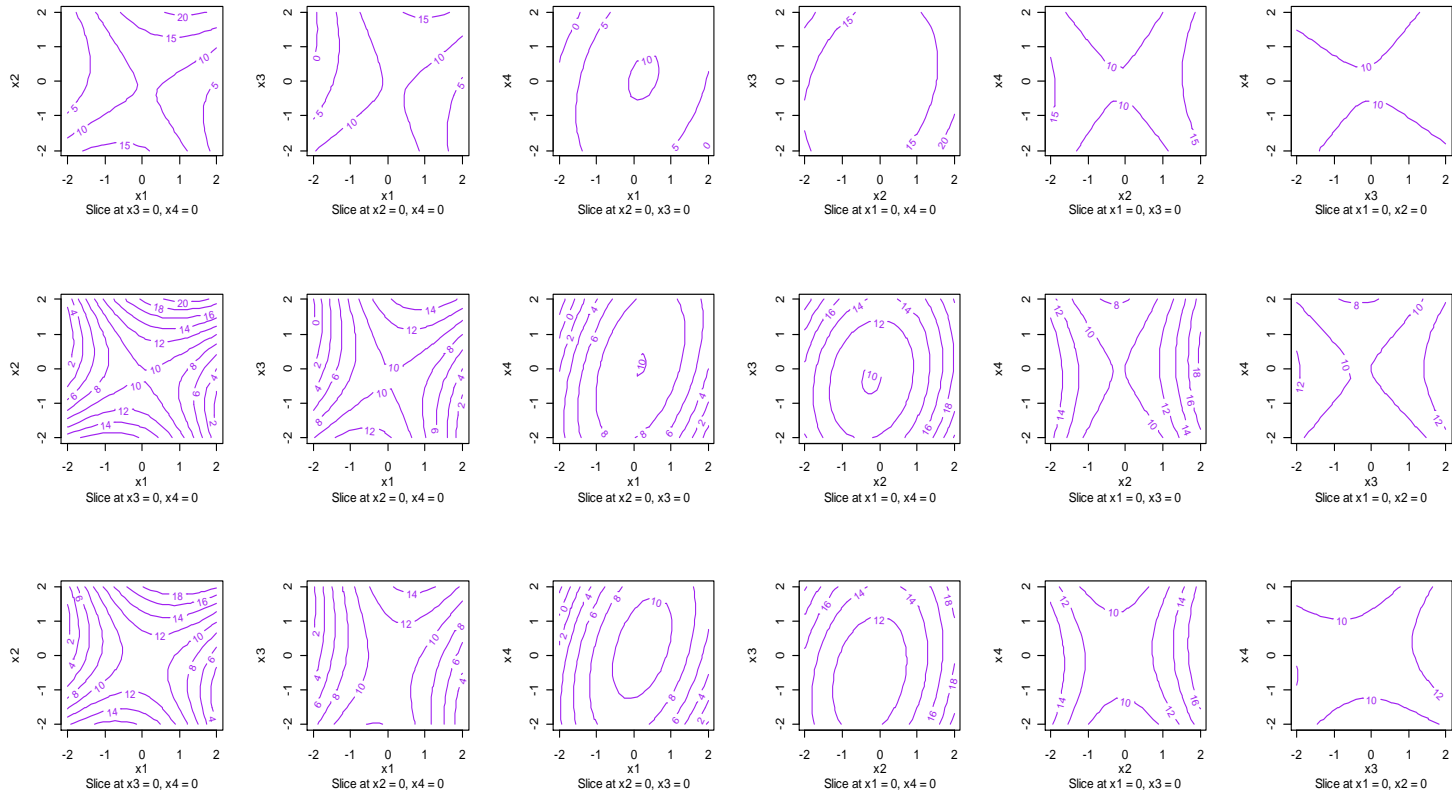


Figure 6: Contour Plot for the Saddle Response Model

Application to the Germination of *Melia volkensii* Experiment

Description of the Germination of *Melia volkensii* Experiment

A four factor rotatable central composite design was used in this experiment. The factors under investigation were temperature, soil PH, concentration of potassium nitrate (KNO_3) and length of time the seeds were soaked in KNO_3 . The experiment was performed by soaking 20 seeds of *Melia* in a solution of KNO_3 for a specified period of time. They seeds were then placed in a petri-dish containing soil of a particular pH. They were then placed in germination chambers of a defined temperature. The outcome was the number of seeds that germinated in a particular petri-dish. The objective was to find the temperature, soil pH, concentration of KNO_3 and pre-treatment time that maximize the germination of *Melia* seeds.

The results of the experiment are presented in table 11.

Table 11: Germination of Melia Experiment Data

Raw Values				Coded Values				Response
Temp. (°C)	Soil PH	Concentration	Pre-treatment Time (Hours)	x_1	x_2	x_3	x_4	y
20	5	0.2	6	-1	-1	-1	-1	4
30	5	0.2	6	1	-1	-1	-1	3
20	9	0.2	6	-1	1	-1	-1	5
30	9	0.2	6	1	1	-1	-1	1
20	5	0.4	6	-1	-1	1	-1	3
30	5	0.4	6	1	-1	1	-1	6
20	9	0.4	6	-1	1	1	-1	6
30	9	0.4	6	1	1	1	-1	5
20	5	0.2	10	-1	-1	-1	1	1
30	5	0.2	10	1	-1	-1	1	6
20	9	0.2	10	-1	1	-1	1	3
30	9	0.2	10	1	1	-1	1	4
20	5	0.4	10	-1	-1	1	1	0
30	5	0.4	10	1	-1	1	1	5
20	9	0.4	10	-1	1	1	1	4
30	9	0.4	10	1	1	1	1	10
15	7	0.3	8	-2	0	0	0	0
35	7	0.3	8	2	0	0	0	3
25	3	0.3	8	0	-2	0	0	1
25	11	0.3	8	0	2	0	0	4
25	7	0.1	8	0	0	-2	0	7
25	7	0.5	8	0	0	2	0	6
25	7	0.3	4	0	0	0	-2	7
25	7	0.3	12	0	0	0	2	8
25	7	0.3	8	0	0	0	0	5
25	7	0.3	8	0	0	0	0	8
25	7	0.3	8	0	0	0	0	12
25	7	0.3	8	0	0	0	0	10
25	7	0.3	8	0	0	0	0	7
25	7	0.3	8	0	0	0	0	11

Analysis of the Germination of *Melia volkensii* Experiment

The characteristics of the fitted models are summarized in tables 12 and 13.

Table 12: The Fitted Germination of *Melia volkensii* Model

	Coefficient	Standard Error	t value	p value
(Intercept)	8.833	0.732	12.075	0.000
Temperature	0.833	0.366	2.278	0.038
Soil pH	0.667	0.366	1.823	0.088
Concentration	0.417	0.366	1.139	0.273
Time	0.083	0.366	0.228	0.823
Temperature ²	-1.896	0.342	-5.541	0.000
Temperature: Soil pH	-0.625	0.448	-1.395	0.183
Temperature: Concentration	0.750	0.448	1.674	0.115
Temperature: Time	1.250	0.448	2.790	0.014
Soil pH ²	-1.646	0.342	-4.810	0.000
Soil pH :Concentration	0.750	0.448	1.674	0.115
Soil pH : Time	0.500	0.448	1.116	0.282
Concentration ²	-0.646	0.342	-1.888	0.079
Concentration: Time	-0.125	0.448	-0.279	0.784
Time ²	-0.396	0.342	-1.157	0.265
Multiple R^2	0.8317			
Adjusted R^2	0.6746			
F statistic	5.2940			
P value	0.0014			

Table 13: Analysis of Variance Table for the Germination of *Melia volkensii* Model

Source	Sum of Squares	Degrees of Freedom	Mean Square	F value	P value
Model	238.000	14	17.000	5.294	0.001
First Order	31.667	4	7.917	2.465	0.090
Two way interaction	53.500	6	8.917	2.777	0.051
Pure Quadratic	152.833	4	38.208	11.899	0.000
Residuals	48.167	15	3.211		
Lack of fit	13.333	10	1.333	0.191	0.987
Pure error	34.833	5	6.967		
Total	286.167	29			

The p value of 0.001 indicated that the model was significant. Further, the adjusted R^2 value showed that 67.5% of the variability in the response was attributable to the model. The stationary point, eigenvalues and the canonical equivalent model are shown in table 14:

Table 14: Stationary point and Eigenvalues for the Germination of *Melia volkensii* Model

Stationary Points				Eigenvalues			
x_1	x_2	x_3	x_4				
0.869	0.507	0.962	1.646	-0.134	-0.511	-1.463	-2.476

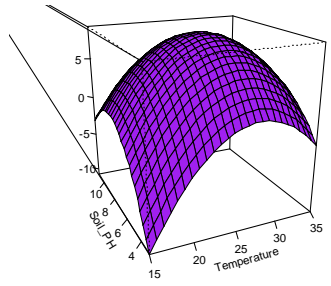
Since all the eigenvalues were negative, the response surface was a maximum one.

The canonical equivalent form of the fitted *Melia volkensii* model was:

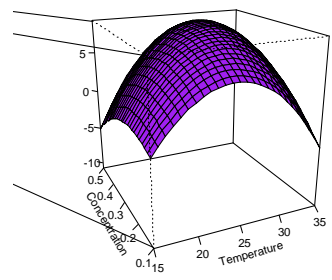
$$\hat{y} = 9.633 - 0.134w_1^2 - 0.511w_2^2 - 1.463w_3^2 - 2.476w_4^2 \quad (34)$$

The stationary point for the model was 0.869, 0.507, 0.962, 1.646. In terms of the natural variable this was 29.35, 8.01, 0.40, 11.29. Thus the optimal temperature was 29.35°C, the optimal soil PH was 8.01, the optimal concentration of KNO_3 was 0.40% and the optimal pre-treatment time is 11.29 hours.

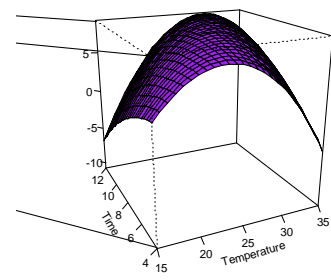
The nature of the response is displayed in figure 7 and figure 8.



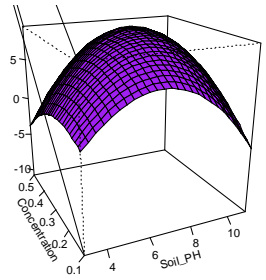
Slice at Concentration = 0.3, Time = 8



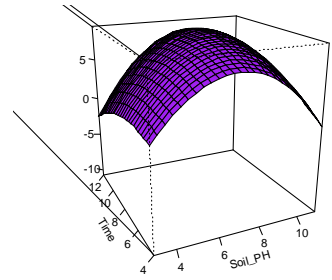
Slice at Soil_PH = 7, Time = 8



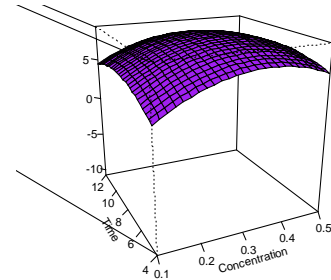
Slice at Soil_PH = 7, Concentration = 0.3



Slice at Temperature = 25, Time = 8



Slice at Temperature = 25, Concentration = 0.3



Slice at Temperature = 25, Soil_PH = 7

Figure 7: Response Surface Plot for the Germination of *Melia volkensii* Model

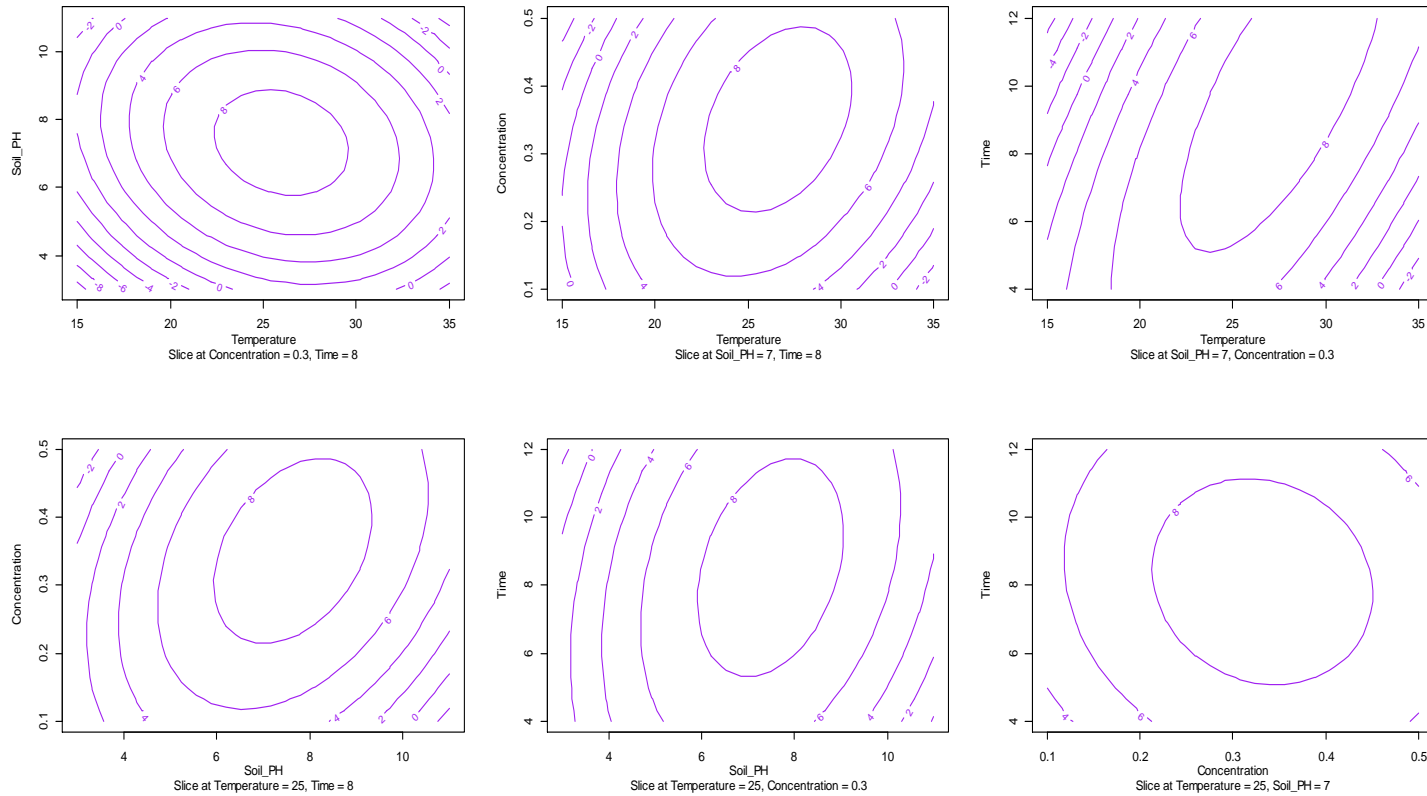


Figure 8: Contour Plot for the Germination of *Melia volkensii* Model

Suppose the investigator was interested in finding where to run the experiment to obtain a response that was close to 9 as possible. This could be obtained from the canonical equivalent model (34).

Letting $\hat{y} = 9$ gives

$$0.134w_1^2 + 0.511w_2^2 + 1.463w_3^2 + 2.476w_4^2 = 0.633 \quad (35)$$

This region can be presented as a contour plot in figure 8

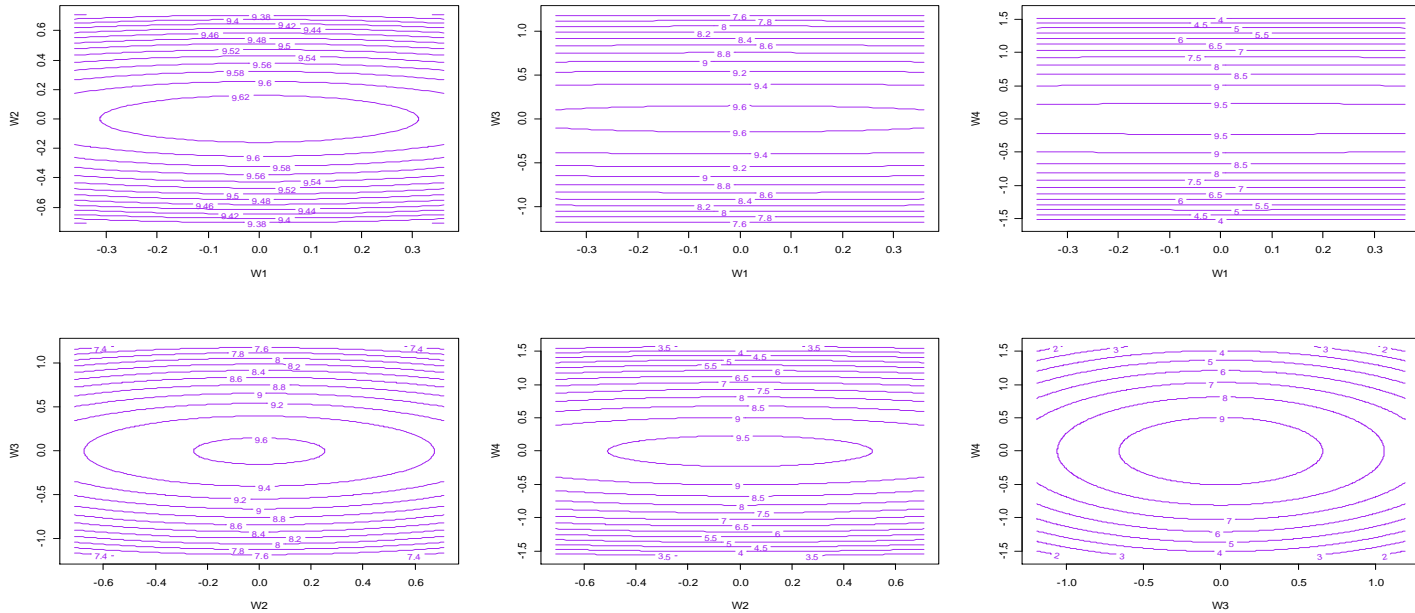


Figure 9: Contour Plot for Expected Response of 9

From (21)

$$\begin{bmatrix} x_1 - x_{1s} \\ x_2 - x_{2s} \\ x_3 - x_{3s} \\ x_4 - x_{4s} \end{bmatrix} = \begin{bmatrix} m_{11} & m_{21} & m_{31} & m_{41} \\ m_{12} & m_{22} & m_{32} & m_{42} \\ m_{13} & m_{23} & m_{33} & m_{43} \\ m_{14} & m_{24} & m_{34} & m_{44} \end{bmatrix}^{-1} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} \quad (36)$$

In this case

$$\begin{bmatrix} m_{11} & m_{21} & m_{31} & m_{41} \\ m_{12} & m_{22} & m_{32} & m_{42} \\ m_{13} & m_{23} & m_{33} & m_{43} \\ m_{14} & m_{24} & m_{34} & m_{44} \end{bmatrix} = \begin{bmatrix} m_{11} & m_{21} & m_{31} & m_{41} \\ m_{12} & m_{22} & m_{32} & m_{42} \\ m_{13} & m_{23} & m_{33} & m_{43} \\ m_{14} & m_{24} & m_{34} & m_{44} \end{bmatrix}^{-1}, \begin{bmatrix} x_{1s} \\ x_{2s} \\ x_{3s} \\ x_{4s} \end{bmatrix} = \begin{bmatrix} 0.869 \\ 0.507 \\ 0.962 \\ 1.646 \end{bmatrix} \text{ Thus}$$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0.869 \\ 0.507 \\ 0.962 \\ 1.646 \end{bmatrix} + \begin{bmatrix} 0.345 & 0.137 & 0.244 & 0.896 \\ -0.061 & -0.220 & -0.923 & 0.309 \\ 0.538 & -0.826 & 0.123 & -0.114 \\ -0.766 & -0.501 & 0.270 & 0.299 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} \quad (37)$$

$$x_1 = 0.869 + 0.345w_1 + 0.137w_2 + 0.244w_3 + 0.896w_4 \quad (38)$$

$$x_2 = 0.507 - 0.061w_1 - 0.220w_2 - 0.923w_3 + 0.309w_4 \quad (39)$$

$$x_3 = 0.962 + 0.538w_1 - 0.826w_2 + 0.123w_3 - 0.114w_4 \quad (40)$$

$$x_4 = 1.646 - 0.766w_1 - 0.501w_2 + 0.270w_3 + 0.299w_4 \quad (41)$$

The table 15 gives values of $w_1, w_2, w_3, w_4, x_1, x_2, x_3$ and x_4 for which $0.134w_1^2 + 0.511w_2^2 + 1.463w_3^2 + 2.476w_4^2 = 0.633$. When the experiment was run at the given values of the temperature, soil PH, concentration of KNO_3 and pre-treatment time the expected response was close to 9.

Table 15: Operating Conditions for Expected Response of 9

w_1	w_2	w_3	w_4	x_1	x_2	x_3	x_4	Tem p.	Soil PH	Con c.	Tim e	\hat{y}
-	-	-	-	0.20	0.87	1.01	1.61	26.0			11.2	8.
0.2	0.2	0.5	0.5	3	0	5	5	1	8.74	0.40	3	2
				0.34	0.84	1.23	1.30	26.7			10.6	8.
0.2	0.2	0.5	0.5	1	6	0	9	0	8.69	0.42	2	6
				0.25	0.78	0.68	1.41	26.2			10.8	8.
0.2	0.2	0.5	0.5	7	2	5	5	9	8.56	0.37	3	5
				0.39	0.75	0.90	1.10	26.9			10.2	8.
0.2	0.2	0.5	0.5	5	8	0	8	8	8.52	0.39	2	8
				-	-	-	-	-	-	-	-	-
-	-		-	0.44	0.05	1.13	1.88	27.2			11.7	7.
0.2	0.2	0.5	0.5	7	3	8	5	3	6.89	0.41	7	8
				-	-	-	-	-	-	-	-	-
				0.58	0.07	1.35	1.57	27.9			11.1	8.
0.2	0.2	0.5	0.5	5	7	3	9	2	6.85	0.44	6	0
				-	-	-	-	-	-	-	-	-
-			-	0.50	0.14	0.80	1.68	27.5			11.3	8.
0.2	0.2	0.5	0.5	1	1	8	5	1	6.72	0.38	7	1
				-	-	-	-	-	-	-	-	-
				0.63	0.16	1.02	1.37	28.2			10.7	8.
0.2	0.2	0.5	0.5	9	5	3	8	0	6.67	0.40	6	3
				1.09	1.17	0.90	1.91	30.4			11.8	8.
-	-	-		1.09	1.17	0.90	1.91	30.4			11.8	8.
0.2	0.2	0.5	0.5	9	9	1	4	9	9.36	0.39	3	3
				1.23	1.15	1.11	1.60	31.1			11.2	8.
0.2	0.2	0.5	0.5	7	5	6	8	8	9.31	0.41	2	1
				1.15	1.09	0.57	1.71	30.7			11.4	8.
-				1.15	1.09	0.57	1.71	30.7			11.4	8.
0.2	0.2	0.5	0.5	3	1	1	4	7	9.18	0.36	3	0
				1.29	1.06	0.78	1.40	31.4			10.8	7.
0.2	0.2	0.5	0.5	1	7	6	7	6	9.13	0.38	1	8
				1.34	0.25	1.02	2.18	31.7			12.3	8.
-	-			1.34	0.25	1.02	2.18	31.7			12.3	8.
0.2	0.2	0.5	0.5	3	6	4	4	1	7.51	0.40	7	8
				1.48	0.23	1.23	1.87	32.4			11.7	8.
0.2	0.2	0.5	0.5	1	2	9	8	0	7.46	0.42	6	5
				1.39	0.16	0.69	1.98	31.9			11.9	8.
-				1.39	0.16	0.69	1.98	31.9			11.9	8.
0.2	0.2	0.5	0.5	7	8	4	4	9	7.34	0.37	7	6
				1.53	0.14	0.90	1.67	32.6			11.3	8.
0.2	0.2	0.5	0.5	5	4	9	7	8	7.29	0.39	5	2

SUMMARY AND CONCLUSIONS

A comprehensive analysis of the four factor second order model was undertaken as reported in this paper. Cases for the three possible responses surfaces namely maximum response, minimum response and saddle response were considered. Additionally a practical experiment scenario was presented. The paper is therefore handy for researchers faced with the challenge of obtaining optimal values of four predictor variables when the response variable exhibits curvilinear behaviour. The work here can

be extended with some appropriate modifications to any number of independent variables.

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