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On the use of nonparametric regression model in Response Surface Methodology

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Abstract. The modeling phase of response surface methodology (RSM) involves the use of regression models to estimate the functional relationship between the response and the explanatory variables using data obtained from a suitable experimental design. In RSM, the Ordinary Least Squares (OLS) is traditionally used to model the data via user-specified low-order polynomials. The OLS model is found to perform poorly if the constant variance (homoscedasticity) assumption is violated. Additionally, the specified polynomials are usually found inadequate for the data. The problems resulting from model inadequacy include biased estimates of the mean response function. Recently, nonparametric regression model, such as the Local Linear Regression (LLR), has been proposed to address the model inadequacy issue associated with the use of the OLS model. The LLR model is flexible, hence, can capture local trend and structure in the data that are misspecified by an inadequate OLS model. The successful application of the LLR model has been limited to studies with three unique features, namely: a single explanatory variable, fairly large sample sizes and space-filling designs. Therefore, the LLR model is scantily used in RSM which general underpinning include economy of data points (small sample size), typically sparse data, and oftentimes, more than one explanatory variables.In this paper, we propose a new nonparametric regression models that incorporate the smoothing of residuals to provide a second opportunity of fitting part of the data that is not captured by the LLR model. Using an example from RSM literature, it is observed that the goodness-of-fits of the proposed model are considerably better when compared with those of the OLS and the LLR models.

Keywords: response surface, local linear regression, ordinary least squares, locally adaptive bandwidths, mixing parameter.

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1. Introduction

Response Surface Methodology (RSM) is a sequential statistical tool employed by statistician and engineers for empirical model building, such that the response variable is optimized (Nair et al., 2014). RSM consists of three main phases namely, experimental design phase, modeling phase and the optimization phase of the fitted regression models. The peculiarity of RSM data which include, small sample size, sparse data and curse of dimensionality have reduced the performance of nonparametric regression models in terms of goodness of fit statistics and optimization result.

Consider the parametric regression model:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \tag{1}$$

where $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}_{(n\times 1)}$ is the vector of response, $\mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix}_{(n\times(k+1))}$ is the model

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matrix, $\mathbf{X} = \mathbf{X}^{(OLS)}$, $\boldsymbol{\epsilon}$ is the vector of error term. The estimated responses for the ith data points are:

$$\hat{\mathbf{y}}_i^{OLS} = \mathbf{x}_i^{'OLS}\left(\mathbf{X}^{'OLS}\mathbf{X}^{OLS}\right)^{-1}\mathbf{X}^{'OLS}\mathbf{y}, i = 1, 2, \cdots, n. \tag{2}$$

In matrix form, equation (2) is expressed as:

$$\hat{\mathbf{y}}^{(OLS)} = \mathbf{H}^{(OLS)}\mathbf{y} = \begin{bmatrix} h_1^{(OLS)} \\ h_2^{(OLS)} \\ \vdots \\ h_n^{(OLS)} \end{bmatrix}\mathbf{y}, \tag{3}$$

where the $1 \times n$ vector $h_i^{(OLS)}$ is the ith row of the $n \times n$ OLS Hat matrix. The drawback of the parametric regression model is that if misspecified, the estimates are usually biased (Swamy et al., 2008; Fathi et al., 2011).

1.1 *The Local Linear Regression Model (LLR)*

Using the weighted least squares theory (Pickle, 2016), the LLR estimator $\hat{y}_i^{(LLR)}$ is given as:

$$\hat{\mathbf{y}}_i^{LLR} = \mathbf{x}_i^{'(LLR)}\left(\mathbf{X}^{'(LLR)}\mathbf{W}_i\mathbf{X}^{(LLR)}\right)^{-1}\mathbf{X}^{'(LLR)}\mathbf{W}_i\mathbf{y}, \qquad i = 1, 2, \cdots, n. \tag{4}$$

where $X^{(LLR)}$ is the LLR model matrix that depends solely on the number of explanatory variables utilized in the experiment, $W_i = W^{Raw}$ is the raw diagonal matrix of kernel(Gaussian) weight used in the estimation of the ith response and $x_i^{'(LLR)}$ is the ith row of the LLR model matrix. In terms of locations, the LLR estimator is expressed as:

$$\hat{\mathbf{y}}_i^{LLR} = \mathbf{h}_i^{'(LLR)}\mathbf{y}, \qquad i = 1, 2, \cdots, n. \tag{5}$$

The drawback of LLR model is that it suffers high bias in regions where the data exhibit curvature (Hastie et al., 2009; Rivers, 2009).

1.2 *Bandwidths for nonparametric regression model*

The choice of bandwidth for nonparametric regression models is a critical criterion and challenging in regression analysis (Kai, 2009; Aydin et al., 2013). Bandwidth selection was designed to minimize bias and variance of the estimate (Rivers, 2009).

A bandwidth b, is said to be fixed if it's value is constant for all the locations in a given regression technique, otherwise it is referred to as locally adaptive bandwidths (Prewitt and Lohr, 2006).

Hence, the kernel function, $K(.)$ employed in RSM is the simplified Gaussian kernel given in Wan and Birch (2011) as:

$$K\left(\frac{x_i - x_0}{b}\right) = K\left(\frac{x_0 - x_i}{b}\right) = \exp\left(\frac{x_i - x_0}{b}\right)^2, \qquad i = 1, 2, \cdots, n. \tag{6}$$

where the kernel weights w_{i0} in the kernel weight matrix is given as:

$$w_{i0} = \frac{K((x_i - x_o)/b)}{\sum_{j=1}^{n} K((x_j - x_o)/b)}, i = 1, 2, \cdots, n. \tag{7}$$

According to Wan (2007), $K\left(\frac{x_i - x_0}{b}\right)$ in equation (6) is referred to as kernel function which regulates

the shape of the kernel weights (e.g. Gaussian kernel), x_0 is a dummy known as target point, b is the bandwidth.

A situation where more than one explanatory variable are used in the model matrix $\mathbf{X}^{(LLR)}$, the kernel weight w_{i0} is a product from simplified Gaussian kernel given as:

$$w_{io} = \prod_{j=1}^{k} K\left(\frac{x_{ij} - x_0}{b}\right) / \sum_{p=1}^{n}\left[\prod_{j=1}^{k} K\left(\frac{x_{pj} - x_0}{b}\right)\right], \qquad i = 1, 2, \cdots, n. \tag{8}$$

(Mays et al., (2001) and Pickle, (2006)). For data originated from RSM, the vector of optimal bandwidths $\Phi = [b_1^*, b_2^*, \cdots, b_n^*]$ is obtained based on the minimization of the Penalized Prediction Error Sum of Squares (PRESS**) (Wan and Birch, 2011). The PRESS** criterion for selecting the bandwidths is given as:

$$\text{PRESS}^{**}(\Phi) = \frac{\sum_{i=1}^{n}\left(y_i - \hat{y}_{i,-i(.)}\right)^2}{n - trace(H^{(.)}(\Phi)) + (n-k-1)\frac{SSE_{max} - SSE_{\Phi}}{SSE_{max}}}, \tag{9}$$

where SSE_{max} is the maximum Sum of Squared Errors obtained as the $b_1, b_2, \cdots, b_n$ approaches infinity, SSE_{Φ} is the sum of squared errors associated with a set of bandwidths $b_1, b_2, \cdots, b_n$, $trace(H^{(.)}(\Phi))$ is the trace of the Hat matrix and $\hat{y}_{i,-i(.)}$ is the leave-one-out cross-validation estimated value of y_i with the ith observation left out (Mays et al. 2001; Wan and Birch 2011).

1.3 *Locally adaptive bandwidths*

Edionwe et al. (2016) proposed locally adaptive bandwidths:

$$b_i = \frac{b^* N\left(C\left[\sum_{j=1}^{n} y_j\right] - y_i\right)}{(Cn-1)\sum_{j=1}^{n} y_j}, \qquad i = 1, 2, \cdots, n \tag{10}$$

where b^* is a fixed optimal bandwidth, y_i, $i = 1, 2, \cdots, n$, could be taken as any statistics that mirrors the insufficiencies in the OLS estimates of the responses, $T = \sum_{j=1}^{n} y_j$, $N > 0$, and $C \geq 0$, are parameters introduced to address the problem of clustering within the interval $[0, 1]$. The optimal chosen tuning parameters of N and C are hereafter refers to as N^* and C^*, respectively.

2. Materials and method

The nonparametric regression model is not restricted to a user specified form as in the parametric counterpart. In spite of its flexibility, nonparametric regression models are challenged in a study such as RSM due to three important aspects in RSM namely;

- Sparseness of RSM data
- Cost efficient design (small sample sizes)
- The study utilizes more than one explanatory variable (a term referred to as curse of dimensionality).

2.1 *Proposed Nonparametric Regression Model (PNRM)*

Let G_i be the sum of Local Polynomial Regression (LPR) of order 1 and the correction term A_i for location i, given by

$$G_i = g_i^{(d)} + A_i, \qquad i = 1, 2, \cdots, n; \qquad d = \text{order of the polynomial} \tag{11}$$

$$= g_i^{(1)} + A_i$$

where $G_i = y_i^{(PNRM)}$, $g_i^{(1)} = y_i^{(LLR)}$, $A_i = \lambda \mathbf{r}_i$, $\lambda \in [0,1]$.λ is the mixing parameter that controls the proportion of the residuals that needed to be added to the component fit of LLR, $\mathbf{r}_i$ are vectors of ith residuals from the fitted LLR. Thus,

$$y_i^{(PNRM)} = y_i^{(LLR)} + \lambda \mathbf{r}_i, \qquad i = 1, 2, \cdots, n. \tag{12}$$

$$E(y_i^{(PNRM)}) = E(y_i^{(LLR)} + \lambda \mathbf{r}_i). \tag{13}$$

The estimators of the component part of Equation (13) are given as:

$$\hat{y}_i^{(PNRM)} = \hat{y}_i^{(LLR)} + \lambda \hat{\mathbf{r}}_i, \tag{14}$$

where $\hat{\mathbf{r}}_i = \hat{\mathbf{r}}_i^{(LLR)}$, $\hat{\mathbf{r}}_i^{(LLR)}$ is the LLR residual fit, $\hat{y}_i^{(LLR)} = h_i^{(LLR)} y_i$ and $\hat{\mathbf{r}}_i^{(LLR)} = h_i^{(LLR)} r_i$, $r_i = [y_i - \hat{y}_i^{(LLR)}]$, $\qquad i = 1, 2, \cdots, n.$

$$\hat{y}_i^{(PNRM)} = \hat{y}_i^{(LLR)} + \lambda h_i^{(LLR)} [y_i - \hat{y}_i^{(LLR)}] \tag{15}$$

$$\hat{\mathbf{y}}_i^{PNRM} = \mathbf{x}_i^{'(LLR)} \left(\mathbf{X}^{'(LLR)} \mathbf{W}_i \mathbf{X}^{(LLR)} \right)^{-1} \mathbf{X}^{'(LLR)} \mathbf{W}_i y + \lambda \mathbf{x}_i^{'(LLR)} \left(\mathbf{X}^{'(LLR)} \mathbf{W}_i^* \mathbf{X}^{(LLR)} \right)^{-1} \times$$

$$\mathbf{X}^{'(LLR)} \mathbf{W}_i^* \left(\mathbf{y} - \mathbf{x}_i^{'(LLR)} \left(\mathbf{X}^{'(LLR)} \mathbf{W}_i \mathbf{X}^{(LLR)} \right)^{-1} \mathbf{X}^{'(LLR)} \mathbf{W}_i \mathbf{y} \right)$$

$$\hat{\mathbf{y}}_i^{PNRM} = \mathbf{x}_i^{'(LLR)} \left(\mathbf{X}^{'(LLR)} \mathbf{W}_i \mathbf{X}^{(LLR)} \right)^{-1} \mathbf{X}^{'(LLR)} \mathbf{W}_i \mathbf{y} + \lambda \mathbf{x}_i^{'(LLR)} \left(\mathbf{X}^{'(LLR)} \mathbf{W}_i^* \mathbf{X}^{(LLR)} \right)^{-1} \times$$

$$\mathbf{X}^{'(LLR)} \mathbf{W}_i^* \left[\mathbf{I} - \mathbf{x}_i^{'(LLR)} \left(\mathbf{X}^{'(LLR)} \mathbf{W}_i \mathbf{X}^{(LLR)} \right)^{-1} \mathbf{X}^{'(LLR)} \mathbf{W}_i \right] \mathbf{y} \tag{16}$$

Using matrix notation, the PNRM can be expressed as:

$$\hat{\mathbf{y}}^{(PNRM)} = \begin{bmatrix} \mathbf{h}_1^{(LLR)} \mathbf{y} + \lambda \mathbf{h}_1^{(LLR)} \left(\mathbf{y} - (\mathbf{h}_1^{(LLR)} \mathbf{y}) \right) \\ \mathbf{h}_2^{(LLR)} \mathbf{y} + \lambda \mathbf{h}_2^{(LLR)} \left(\mathbf{y} - (\mathbf{h}_2^{(LLR)} \mathbf{y}) \right) \\ \vdots \\ \mathbf{h}_n^{(LLR)} \mathbf{y} + \lambda \mathbf{h}_n^{(LLR)} \left(\mathbf{y} - (\mathbf{h}_n^{(LLR)} \mathbf{y}) \right) \end{bmatrix} \tag{17}$$

$$\hat{\mathbf{y}}^{(PNRM)} = \begin{bmatrix} \mathbf{h}_1^{(LLR)} + \lambda \mathbf{h}_1^{(LLR)} \left(\mathbf{I} - (\mathbf{h}_1^{(LLR)}) \right) \\ \mathbf{h}_2^{(LLR)} + \lambda \mathbf{h}_2^{(LLR)} \left(\mathbf{I} - (\mathbf{h}_2^{(LLR)}) \right) \\ \vdots \\ \mathbf{h}_n^{(LLR)} + \lambda \mathbf{h}_n^{(LLR)} \left(\mathbf{I} - (\mathbf{h}_n^{(LLR)}) \right) \end{bmatrix} \mathbf{y} \tag{18}$$

$$\hat{\mathbf{y}}^{(PNRM)} = \mathbf{H}^{(PNRM)} \mathbf{y}, \tag{19}$$

where $\mathbf{W}_i^* = \mathbf{W}^{Resid}$ is an $n \times n$ diagonal weights matrix for estimating the ith LLR residual, $\mathbf{I}$ is the $n \times n$ identity matrix, the $1 \times n$ vector $\left[\mathbf{h}_i^{(LLR)} + \lambda \mathbf{h}_i^{(LLR)} \left(\mathbf{I} - (\mathbf{h}_i^{(LLR)})\right)\right]$ is the ith row of the PNRM Hat matrix, $\mathbf{H}^{(PNRM)}$. $W_i = W^{Raw}$ is an $n \times n$ raw diagonal matrix of the kernel weights for estimating the ith response. The matrix W_i is given as:

$$\mathbf{W}_i = \begin{bmatrix} w_{i1} & 0 & \cdots & 0 \\ 0 & w_{i2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w_{in} \end{bmatrix}, i = 1, 2, \cdots, n. \tag{20}$$

The parameter λ, is known as the mixing parameter whose optimal value λ^* is selected based on the minimization of the $PRESS^{**}$ criterion:

$$\text{PRESS}^{**}(\lambda) = \frac{\sum_{i=1}^{n} \left(y_i - \hat{y}_{i,-i(\Phi,\lambda)}\right)^2}{n - trace(H^{(\cdot)}(\Phi, \lambda)) + (n-k-1)\frac{SSE_{max} - SSE_{\Phi}}{SSE_{max}}}, \tag{21}$$

where $\Phi = [b_1^*, b_2^*, \cdots, b_n^*]$ is the vector of optimal bandwidths, SSE_{Φ} is the Sum of Squared Errors associated with the set of the optimal bandwidths, $[b_1^*, b_2^*, \cdots, b_n^*]$, $trace(H^{(\cdot)}(\Phi, \lambda))$ is the trace of Hat matrix, and $y_{i,-i}^{(\cdot)}(\Phi, \lambda)$ is the leave-one-out cross-validation estimate of y_i.

2.2 *Algorithm I: Leave – One – Out cross validation procedures for selecting bandwidths and mixing parameter for the proposed model*

Step 1: obtain the bandwidth b_i for location i

$$b_i = \frac{b^* N \left(C \left[\sum_{j=1}^{n} y_j\right] - y_i\right)}{(Cn-1)\sum_{j=1}^{n} y_j}, \qquad i = 1, 2, \cdots, n.$$

Step 2: Define a set H of permissible values of bandwidths (for RSM data, H $\in (0, 1]$) from where the bandwidths b_i, $i = 1, 2, \cdots, n$ are assigned values.
Step 3: Construct the leave-one-out cross validation:

$$\text{PRESS}^{**}(b) = \frac{\sum_{i=1}^{n} \left(y_i - \hat{y}_{i,-i(\Phi)}\right)^2}{n - trace(H^{(\cdot)}(\Phi)) + (n-k-1)\frac{SSE_{max} - SSE_{\Phi}}{SSE_{max}}},$$

for selecting bandwidths on the interval $(0, 1]$ and obtain $y_{i,-i}(\Phi)$ the estimated response at location i, leaving out the ith observation for the set of adaptive bandwidths $\Phi = [b_1, b_2, \cdots, b_n; b_1, b_2, \cdots, b_n; b_1^*, b_2^*, \cdots, b_n^*]$.
Step 4: obtain SSE_{max} as $\mathbf{b}$ tends to infinity, (say $b = 1000000000000000000$) in $\hat{\mathbf{y}}_i^{(LLR)}(\mathbf{b})$

$$SSE_{max} = \sum_{i=1}^{n} \left(\mathbf{y}_i - \hat{\mathbf{y}}_i^{(LLR)}(b)\right)^2$$

Step 5: obtain SSE_{Φ} for a set of adaptive bandwidths:

$$SSE_{\Phi}(b_1, b_2, \cdots, b_n) = \sum_{i=1}^{n} \left(\mathbf{y}_i - \hat{\mathbf{y}}_i^{(LLR)}(b_1, b_2, \cdots, b_n)\right)^2.$$

Step 6: obtain the mixing parameter λ via $PRESS^{**}$

$$\text{PRESS}^{**}(\lambda) = \frac{\sum_{i=1}^{n}\left(y_i - \hat{y}_{i,-i(\Phi,\lambda)}\right)^2}{n - trace(H^{(\cdot)}(\Phi,\lambda)) + (n-k-1)\frac{SSE_{max}-SSE_{\Phi}}{SSE_{max}}}.$$

2.3 *Algorithm II: Algorithm for the implementation of PNRM*

Step 1: Choose the set of bandwidths and mixing parameter that minimizes $PRESS^{**}$ criterion.
Step 2: Define the proposed model

$$\hat{\mathbf{y}}_i^{(PNRM)} = \hat{\mathbf{y}}_i^{(LLR)} + \lambda \mathbf{h}_i^{(LLR)}\left[\mathbf{y}_i - \hat{\mathbf{y}}_i^{(LLR)}\right]$$

Step 3: carryout a loop for each set of bandwidths and the mixing parameter on $\hat{\mathbf{y}}_i^{(PNRM)}$ at location $i = 1(1)n$.
Step 4: STOP

3. Application and discussion of results

The Genetic Algorithm toolbox in Matlab is used to obtain the optimal locally adaptive bandwidths $\hat{\Phi}$ in Equation (10) as well as the optimal mixing parameter, λ^* based on the minimization of PRESS** criterion. A multiple response problem is used in order to compare the statistical performance of the proposed model with the existing OLS and LLR models.

3.1 *The multiple response chemical process data*

The following problem as given in He et al. (2009, 2012) was to obtain the setting of the explanatory variables x_1 and x_2 (representing reaction time and temperature, respectively) that would simultaneously optimize three quality measures of a chemical solution y_1, y_2 and y_3 (representing yield, viscosity, and molecular weight, respectively). The process requirements for each response are as follows:
Maximize y_1 with lower limit $L = 78.5$, with target value $\Phi = 80$; y_2 should take a value in the range $L = 62$ and $U = 68$ with target value $\Phi = 65$; minimize y_3 with upper limit $U = 3300$ with target value $\Phi = 3100$.
Based on the process requirements a Central Composite Design (CCD) was conducted to establish the design experiment and observed responses as presented in Table 1.

3.2 *Desirability function*

The desirability function $d_r(\hat{y}_r(\mathbf{x}))$, $r = 1, 2, \cdots, m$, assigns values between 0 and 1 based on the process requirements such that the most undesirable and desirable values are $d_r(\hat{y}_r(\mathbf{x})) = 0$ and $d_r(\hat{y}_r(\mathbf{x})) = 1$, respectively. Desirability function is applied in Multi-Response Optimization (MRO), where responses are classified as larger the better (LTB) for maximizing the response, smaller the better (STB) for minimizing the response, and nominal the better (NTB) is a two sided transformation of the response (Pickle, 2006; He et al., 2009; 2012).

(1) For Larger-the-Better (LTB) response, $d_1(\hat{y}_1(\mathbf{x}))$ given as:

$$d_1(\hat{y}_1(\mathbf{x})) = \begin{cases} 0 & \hat{y}_1(\mathbf{x}) < 78.5 \\ \left\{\frac{\hat{y}_1(\mathbf{x})-78.5}{80-78.5}\right\}^{t_1} & 78.5 \le \hat{y}_1(\mathbf{x}) \le 80 \\ 1 & \hat{y}_1(\mathbf{x}) > 80 \end{cases} \tag{22}$$

s.t $\mathbf{x} \in [0, 1]$, where the desirability function $d_1(\hat{y}_1(\mathbf{x})) = d_1$ is a scalar measure, $T = 80$ and

Table 1.: Designed experiment and response values

Order	ξ_1	ξ_2	x_1	x_2	y_1	y_2	y_3
1	80	170	-1	-1	76.5	62	2940
2	90	170	1	-1	78.0	66	3680
3	80	180	-1	1	77.0	60	3470
4	90	180	1	1	79.5	59	3890
5	77.93	175	-1.414	0	75.6	71	3020
6	92.07	175	1.414	0	78.4	68	3360
7	85	167.93	0	-1.414	77.0	57	3150
8	85	182.07	0	1.414	78.5	58	3630
9	85	175	0	0	79.9	72	3480
10	85	175	0	0	80.3	69	3200
11	85	175	0	0	80.0	68	3410
12	85	175	0	0	79.7	70	3290
13	85	175	0	0	79.8	71	3500

ξ_1, ξ_2 are natural variables, x_1, x_2 are coded variables and y_1, y_2, y_3 are responses.
Source: He et al. (2009, 2012).

$L = 78.5$ are the maximum acceptable value and lower limit, respectively; t_1 is taken to be 1. The objective is to maximize the response $\hat{y}_1(\mathbf{x})$.

(2) For the Nominal-the-Better (NTB) response, $d_2(\hat{y}_2(\mathbf{x}))$ is a two sided transformation given as:

$$d_2(\hat{y}_2(\mathbf{x})) = \begin{cases} \left\{\frac{\hat{y}_2(\mathbf{x})-62}{65-62}\right\}^{t_2} & 62 \leq \hat{y}_2(\mathbf{x}) < 65 \\ \left\{\frac{68-\hat{y}_2(\mathbf{x})}{68-65}\right\}^{t_2} & 65 \leq \hat{y}_2(\mathbf{x}) \leq 68 \\ 0 & \text{otherwise} \end{cases} \tag{23}$$

s.t $\mathbf{x} \in [0, 1]$, where $d_2(\hat{y}_2(\mathbf{x})) = d_2$, $L = 62$, $U = 68$, $T = 65$ is the target value of the response $\hat{y}_2(\mathbf{x})$. However, for RSM data, the parameters values of t_1 and t_2 are taken to be 1 (Castillo, 2007; Wan, 2007; He et al., 2012).

(3) when the response is of the smaller-the-better (STB) type, $d_3(\hat{y}_3(\mathbf{x}))$ is given as:

$$d_3(\hat{y}_3(\mathbf{x})) = \begin{cases} 1 & \hat{y}_3(\mathbf{x}) < 3100 \\ \left\{\frac{3300-\hat{y}_3(\mathbf{x})}{3300-3100}\right\}^{t_2} & 3100 \leq \hat{y}_3(\mathbf{x}) \leq 3300 \\ 0 & \hat{y}_3(\mathbf{x}) > 3300 \end{cases} \tag{24}$$

s.t $\mathbf{x} \in [0, 1]$,

where $d_3(\hat{y}_3(\mathbf{x})) = d_3$, $T = 3100$ and $U = 3300$ are the minimum acceptable value and upper limit, respectively. The objective is to minimize the response $\hat{y}_3(\mathbf{x})$.

3.3 *The overall desirability*

According to Ramakrishnan and Arumugam (2012), the overall desirability function D(x) is the geometric mean of the individual desirability functions given as:

$$D(\mathbf{x}) = \sqrt[3]{(d_1(\hat{y}_1(\mathbf{x})) \times d_2(\hat{y}_3(\mathbf{x})) \times d_3(\hat{y}_3(\mathbf{x}))} \tag{25}$$

The higher the overall desirability function, $D(\mathbf{x})$, is an indication of a higher overall satisfaction for all responses.

3.4 *Transformation of data from Central Composite Design (CCD)*

Following nonparametric regression procedures in RSM, the values of the explanatory variables are coded between 0 and 1. The data collected via a Central Composite Design (CCD) is transformed by a mathematical relation:

$$x_{new} = \frac{\min(x_{old}) - x_0}{\min(x_{old}) - \max(x_{old})} \tag{26}$$

where x_{new} is the transformed value, x_0 is the target value that needed to be transformed in the vector containing the old coded value, represented as x_{old}, $\min(x_{old})$ and $\max(x_{old})$ are the minimum and maximum values in the vector x_{old} respectively (He et al., 2012). The natural or coded variables in Table 1 can be transformed to explanatory variables in Table 2 using equation (26). Target points needed to be transformed for location 1 under the coded variables are given below:
Target points x_0: -1, -1; $\min(x_{old})$: -1.414, -1.414; $\max(x_{old})$: 1.414, 1.414.

$$x_{new} = \frac{\min(x_{old}) - x_0}{\min(x_{old}) - \max(x_{old})}.$$

$$\text{Explanatory variable } x_1: \qquad x_{11} = \frac{-1.414 - (-1)}{(-1.414) - (1.414)} = 0.1464.$$

$$\text{Explanatory variable } x_2: \qquad x_{12} = \frac{-1.414 - (-1)}{(-1.414) - (1.414)} = 0.1464.$$

Target points needed to be transformed for location 2 under the coded variables are given below:
Target points x_0: 1 ,-1; $\min(x_{old})$: $-1.414, -1.414$; $\max(x_{old})$: $1.414, 1.414$.

$$x_{new} = \frac{\min(x_{old}) - x_0}{\min(x_{old}) - \max(x_{old})}.$$

$$\text{Explanatory variable } x_1: \qquad x_{21} = \frac{(-1.414 - (1))}{((-1.414) - (1.414))} = 0.8536.$$

$$\text{Explanatory variable } x_2: \qquad x_{22} = \frac{(-1.414 - (-1))}{((-1.414) - (1.414))} = 0.1464.$$

Target points needed to be transformed for location 6 under the coded variables are given below:
Target points x_0: 1.414, 0; $\min(x_{old})$: $-1.414, -1.414$; $\max(x_{old})$: $1.414, 1.414$.

$$x_{new} = \frac{\min(x_{old}) - x_0}{\min(x_{old}) - \max(x_{old})}.$$

$$\text{Explanatory variable } x_1: \qquad x_{61} = \frac{-1.414 - (1.414)}{((-1.414) - (1.414))} = 1.0000.$$

$$\text{Explanatory variable } x_2: \qquad x_{62} = \frac{(-1.414 - (0))}{((-1.414) - (1.414))} = 0.5000.$$

Repeating the process up to location 13, then we obtain the entries for explanatory variables x_1 and x_2, respectively, in Table 2.

Table 2.: Chemical Process Transformed Data

i	x_1	x_2	y_1	y_2	y_3
1	0.1464	0.1464	76.5	62	2940
2	0.8536	0.1464	78.0	66	3680
3	0.1464	0.8536	77.0	60	3470
4	0.8536	0.8536	79.5	59	3890
5	0.0000	0.5000	75.6	71	3020
6	1.0000	0.5000	78.4	68	3360
7	0.5000	0.0000	77.0	57	3150
8	0.5000	1.0000	78.5	58	3630
9	0.5000	0.5000	79.9	72	3480
10	0.5000	0.5000	80.3	69	3200
11	0.5000	0.5000	80.0	68	3410
12	0.5000	0.5000	79.7	70	3290
13	0.5000	0.5000	79.8	71	3500

The optimal values of the parameters of the proposed model and the LLR for each response variable are presented in Table 3.

Table 3.: Optimal values of the tuning parameters and mixing parameter of the proposed model and the LLR model for the multiple response chemical process data

	Proposed	Model				LLR	
Response	$\mathbf{N}^*(\mathbf{W}^{Raw})$	$\mathbf{C}^*(\mathbf{W}^{Raw})$	$\mathbf{N}^*(\mathbf{W}^{Resid})$	$\mathbf{C}^*(\mathbf{W}^{Resid})$	λ^*	$\mathbf{N}^*$	$\mathbf{C}^*$
y_1	3.6241	1.2876	3.0413	0.0798	0.9457	3.0971	0.0797
y_2	6.5583	0.1246	1.2854	0.0952	1.0000	1.2297	0.0952
y_3	1.9999	0.0664	1.2050	0.0935	1.0000	4.8181	0.0896

Based on the production requirements for the responses y_i, Table 3 highlights the optimal values of tuning parameters for both raw $\mathbf{N}^*(\mathbf{W}^{Raw})$, $\mathbf{C}^*(\mathbf{W}^{Raw})$, residual ($\mathbf{N}^*(\mathbf{W}^{Resid})$, $\mathbf{C}^*(\mathbf{W}^{Resid})$) as well as the optimal mixing parameter λ^* for the proposed model and the LLR optimal tuning parameters $(\mathbf{N}^*, \mathbf{C}^*)$.

The locally adaptive optimal bandwidths for raw and residual multiple response case for the proposed and LLR models via PRESS** criterion are presented in Tables 4 and 5 respectively.

Table 4.: Locally Adaptive Optimal Bandwidths for the Proposed Model

	Optimal	Bandwidths	for $\mathbf{W}^{Raw}$	Optimal	Bandwidths	for $\mathbf{W}^{Resid}$
i	y_1	y_2	y_3	y_1	y_2	y_3
1	0.2792	0.5475	0.0057	0.3972	0.1209	0.1501
2	0.2789	0.4978	0.2513	0.2733	0.0955	0.0549
3	0.2791	0.5724	0.1816	0.3559	0.1336	0.0819
4	0.2785	0.5848	0.3210	0.1495	0.1400	0.0279
5	0.2794	0.4356	0.0322	0.4715	0.0637	0.1398
6	0.2788	0.4729	0.1451	0.2403	0.0827	0.0961
7	0.2791	0.6097	0.0754	0.3559	0.1527	0.1231
8	0.2788	0.5973	0.2347	0.2320	0.1463	0.0613
9	0.2785	0.4232	0.1849	0.1164	0.0573	0.0806
10	0.2784	0.4605	0.0920	0.0834	0.0764	0.1166
11	0.2784	0.4729	0.1617	0.1082	0.0827	0.0896
12	0.2785	0.4481	0.1218	0.1329	0.0700	0.1051
13	0.2785	0.4356	0.1916	0.1247	0.0637	0.0781

Table 5.: Locally Adaptive Optimal Bandwidths for LLR Model

i	y_1	y_2	y_3
1	0.4045	0.1156	0.6669
2	0.2783	0.0913	0.1755
3	0.3624	0.1278	0.3149
4	0.1522	0.1339	0.0360
5	0.4802	0.0609	0.6138
6	0.2447	0.0792	0.3880
7	0.3624	0.1461	0.5275
8	0.2363	0.1400	0.2087
9	0.1186	0.0548	0.3083
10	0.0849	0.0731	0.4943
11	0.1102	0.0792	0.3548
12	0.1354	0.0670	0.4345
13	0.1270	0.0609	0.2950

The goodness-of-fit of the models for the chemical process data are shown in Table 6.

Table 6.: Goodness-of-fit of the Models for the Chemical Process Data

Response	Model	DF	PRESS**	PRESS	SSE	MSE	R^2	R^2_{Adj}
y_1	OLS	7.0000	0.3361	2.3525	0.4962	0.0709	0.9827	0.9704
	LLR	4.7810	0.2063	3.0148	0.3113	0.0651	0.9892	0.9728
	Proposed	4.7093	0.2046	2.9781	0.2909	0.0618	0.9899	0.9742
y_2	OLS	7.0000	28.8726	202.1082	36.2242	5.1749	0.8997	0.8281
	LLR	4.0000	9.4343	129.4141	10.0000	2.5000	0.9723	0.9170
	Proposed	4.0000	9.0889	124.6763	10.0000	2.5000	0.9723	0.9170
y_3	OLS	7.0000	159080	1113600	207870	29696	0.7590	0.5868
	LLR	5.8380	40779	508170	92621	15865	0.8926	0.7795
	Proposed	4.0000	44326	514370	65720	16430	0.9238	0.7714

The results in Table 6 clearly explain the goodness-of-fit statistics for multiple response chemical process data. Obviously, the proposed model is superior in terms of minimum values for the PRESS** within two responses (y_1 and y_2), minimum SSE across two responses (y_1 and y_3) and a tie with LLR in y_2 and minimum R^2 across the two responses (y_1 and y_3) and a tie with LLR in y_2. Generally, it implies that the proposed model produces a more practical and reliable results in eight cells, and with a joint performance in other four cells, which obviously guarantee for a better model. There is correlation between Table 6 and Figure 1 in terms of the three residual plots for all the data points. The plot for y_1 residual has a slightly better explained variation for the proposed model over LLR, but clearly outperforms the OLS which is also confirmed in Table 6. The data points for y_2 residual coincide between the proposed model and the LLR but differ with the OLS by way of improved explained variation. The data point for the proposed model in y_3 residual has higher explained variation over LLR and OLS. Apparently, these observations indicate that the proposed model offers more accurate fits over LLR and OLS.

Table 7.: Model optimal solution based on the Desirability function for the multiple response chemical process data

Model	x_1	x_2	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_3$	d_1	d_2	d_3	D(%)
OLS	0.4449	0.2226	78.7616	66.4827	3229.9	0.1744	0.5058	0.3504	31.5800
LLR	0.5155	0.3467	78.6965	65.0328	3285.9	0.1310	0.9891	0.0703	20.8837
Proposed model	0.4845	0.3641	78.8072	65.7368	3251.2	0.2048	0.7544	0.2441	33.5343

The overall goal of the desirability function as given in Table 7 is to determine an operating conditions (setting) of the explanatory variables that would simultaneously optimize the responses.

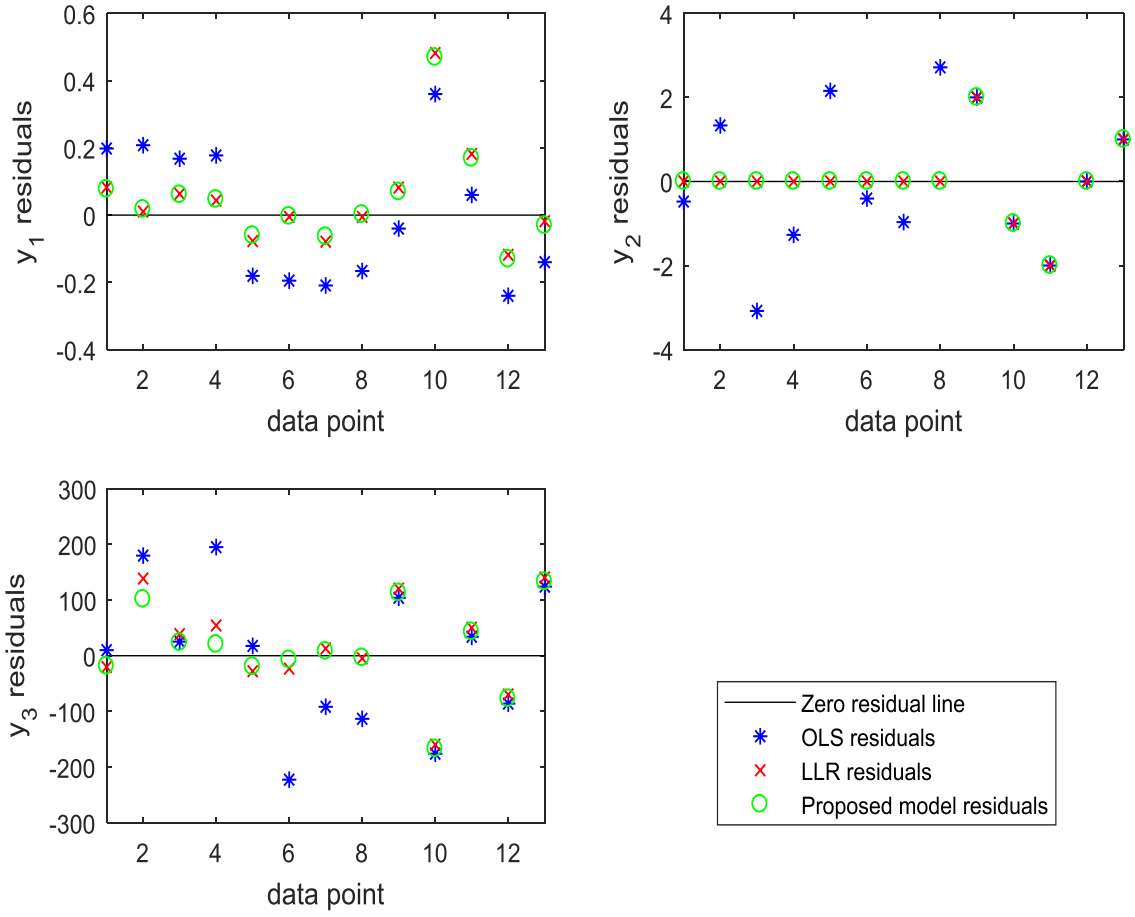

Figure 1.: Plots of Model residuals for the multiple response chemical process data

The operating settings for the proposed model optimize the responses with a higher desirability as compared with LLR and OLS. Therefore, it is established that the contribution from the proposed model satisfies the production requirements over LLR and OLS.

3.5 *Discussion of results*

The results presented in Table 6, shows that PNRM, either completely or conjointly, provides the best results in terms of all the statistics for y_1 and y_2. For the y_3, the PNRM offers the best results in two out of the six statistics for comparison. Interestingly, PNRM gives the best PRESS** in y_1 and y_2. Figure 1 is a reflection of the results presented in Table 6, where the interest is to give a pictorial display of the measure of variability not explained in the data by OLS, LLR and PNRM models for a multiple response problem. The obvious from Figure 1, is that PNRM has less variability compared with OLS and LLR models. Lastly, Table 7, addresses the production or process requirements for each response, such that $\hat{y}_1$ must not be less 78.5, otherwise the desirability $d_1(\hat{y}_1(\mathbf{x}))$ becomes zero. $\hat{y}_2$ must lie between the values 62 and 68 inclusive, otherwise the desirability $d_2(\hat{y}_2(\mathbf{x}))$ takes the value zero. $\hat{y}_3$ must not exceed 3300, otherwise the desirability $d_3(\hat{y}_3(\mathbf{x}))$ is assign a zero. The model with the highest overall desirability, $D(\%)$ has the optimal settings of the explanatory variable that will optimize the responses. Hence, PNRM provides the best settings that optimize the response for the multiple response chemical process data as compared with OLS and LLR models.

4. Conclusion

In this paper, we considered two existing regression models, the OLS and LLR and proposed a nonparametric regression model (PNRM) that utilizes the locally adaptive bandwidths of Edionwe et al. (2016) for smoothing RSM data. The results of the performance statistics obtained from an empirical data and optimal solutions show that the PNRM regression model performs better than OLS and the LLR that utilizes the locally adaptive bandwidths of Edionwe et al., (2016). Therefore, worthy to refer is the remarkable low values of the $PRESS^{**}$ criterion and SSE of the PNRM. This promises high accuracy in predicting yield, viscosity, and molecular weight, for multiple response problems. Lastly, the PNRM in Table 7, display higher level of desirability over OLS and LLR models and as such provided a setting for the explanatory variables that optimized the response for multiple response chemical process data.

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Appendix

Computer Program Written in Matlab Codes for getting Optimal Bandwidths parameters for the Proposed Model via the Genetic Algorithm

Function press=my_proposed_model (N)
Input n by 1 vectors of explanatory variables x_1,x_2,...,x_k written in Matlab as x1, x2,...,xk;
Input n by 1 vector of response y;
Define first column of model matrices for LLR: const=ones(n,1);
Define n by (1+k) model matrix for LLR: X1=[const x_1,x_2,...,x_k];
Assign value to constant e=2.7183;
Assign value to constant n=length(x_1,);
Assign value to constant k=rank(X1)-1;
Assign value to mixing parameter lambda=1.0000 which may be written in Matlab as g=1.0000;
Calculate SSM=sum((y-mean(y)).∧2);
%%%%%%%%%%%%%%%%%%%%%%
Get the value of T in equation (10): T=sum(y);
Define N in equation (16)for getting local bandwidths for raw response N(1);
Define C in equation (16)for getting local bandwidths for raw response N(2);
Define N in equation (16)for getting local bandwidths for LLR residuals N(3);
Define C in equation (16) for getting local bandwidths for LLR residuals N(4);
Define N=[N(1) N(2) N(3) N(4)];
Define the local bandwidths selector in equation (10) for raw response as b1=(N(1)*(N(2)*T-y))/(T*((N(2)*n)-1));
Define the local bandwidths selector in equation (10) for residuals as
b2=(N(3)*(N(4)*T-y))/(T*((N(4)*n)-1));
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%% Preallocate dimension for vectors;
ymax=zeros(n,1);yPNRMcv=zeros(n,1);a=zeros(n,1);yPNRM=zeros(n,1);
%%% Get maximum SSE in equation (9);
Assign large bandwidth for getting maximum SSE: bmax=99999999999999999;
for i=1:n;
%%%%% Get diagonal weights matrices for raw response;
w1max_raw=
((1/e).∧(((x1-x1(i))./bmax).∧2)).*((1/e).∧(((x2-x2(i))./bmax).∧2))· · ·.*((1/e).∧(((xk-xk(i))./bmax).∧2));
WWmax_raw=sum(w1max_raw);

```
kerweight_max_raw=w1max_raw./WWmax_raw;
Wmax_raw=diag(kerweight_max_raw);
%%%%% Get diagonal weights matrices for LLR plus LLR residuals;
w1max_residuals=
((1/e).∧(((x1-x1(i))./bmax).∧2)).*((1/e).∧(((x2-x2(i))./bmax).∧2))· · · .*((1/e).∧(((xk-xk(i))./bmax).∧2));
WWmax_residuals=sum(w1max_residuals);
kerweight_max_residuals=w1max_residuals./WWmax_residuals;
Wmax_residuals=diag(kerweight_max_residuals);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
Define the n by n identity matrix in equation (16) v=eye(n,n);
Define LLR Hat matrix in (16) v2=X1*((X1'*Wmax_raw*X1)1'*Wmax_raw);
Define matrix [ I-x_i∧'(LLR) (X∧'(LLR) W_i X∧((LLR) ) )∧(-1) X∧'(LLR) W_i]] in (16) vt1=v-v2;
%%%% Get the ith row of the n by n PNRM Hat matrix;
Hat_max=
X1(i,:)*((X1'*Wmax_raw*X1)\(X1'*Wmax_raw))+X1(i,:)*((X1'*Wmax_residuals*X1)\(X1'*Wmax_residuals*vt1);
%%%%% Get the PNRM estimate of the response based on bmax;
ymax(i)=Hat_max*y;
end
Calculate SSEmax=sum((y-ymax).∧2);
%%%%%%%%% Get diagonal weights matrices for cross validation and PNRM estimate of response
%%%%%%%%% for optimal bandwidths
for i=1:n;
w1_raw=
((1/e).∧(((x1-x1(i))./b1).∧2)).*((1/e).∧(((x2-x2(i))./b1).∧2))· · · .*((1/e).∧(((xk-xk(i))./b1).∧2));
WW_raw=sum(w1_raw);
kerweight_raw=w1_raw./WW_raw;
%%%%%%%%%%%%%%%%%%%%%%%%%%
w1_residuals=
((1/e).∧(((x1-x1(i))./b2).∧2)).*((1/e).∧(((x2-x2(i))./b2).∧2))· · · .*((1/e).∧(((xk-xk(i))./b2).∧2));
WW_residuals=sum(w1_residuals);
kerweight_residuals=w1_residuals./WW_residuals;
%%%%%%%%%% Delete the ith of the arrays for leave-one-out regression procedure
Kerweight_raw(i,:)=[];
kerweight_residuals(i,:)=[];
y(i,:)=[];
X1(i,:)=[];
Define the diagonal weight matrix for raw response W_raw=diag(kerweight_raw);
Define the diagonal weight matrix for LLR plus LLR residuals
W_residuals=diag(kerweight_residuals);
Define the (n-1) by (n-1) identity matrix v=eye(n-1,n-1);
Define LLR (n-1) by (n-1) Hat matrix v2=X1*((X1'*W_raw*X1)\ X1'*W_raw);
Define matrix [ I- x_i∧'(LLR) (X∧'(LLR) W_i X∧((LLR) ))∧(-1) X∧'(LLR) W_i]] in (16) vt2=v-v2;
Define LLR coefficients for raw response in the ith data point: a2=(X1'*W_raw*X1)\ X1'*W_raw*y;
Define LLR coefficients for residuals in the ith data point:
a3=(X1'*W_residuals*X1)\ X1'*W_residuals*vt2*y;
%%%% Restore original dimensions of arrays
Kerweight_raw=w1_raw./WW_raw;
kerweight_residuals=w1_residuals./WW_residuals;
n by(1+k)vector of LLR model matrix X1=[const x1 x2 ... xk];
n by 1 vector of response y;
%%%%% Get the ith leave-one-out estimates haty _(i,-i)∧((PNRM )) of response y_i, i=1,2,...,n, in equation
(16)
yPNRMcv(i)= X1(i,:)*a2+g*X1(i,:)*a3;
%%%%% Get the ith estimates haty _i∧((PNRM)) of response y_i, i=1,2,. . . ,n.
W_raw=diag(kerweight_raw);
W_residuals=diag(kerweight_residuals);
v=eye(n,n);
v2=X1*((X1'*W_raw*X1)\ X1'*W_raw);
Define matrix [ I- x_i∧'(LLR) (X∧'(LLR) W_i X∧((LLR)))∧(-1) X∧'(LLR) W_i]] in (16) vt3=v-v2;
Hat_PNRM=
X1(i,:)*((X1'*W_raw*X1)\(X1'*W_raw))+g*X1(i,:)*((X1'*W_residuals*X1)\ (X1'*W_residuals*vt3));
Define ith element of the ith row of the PNRM Hat matrix a(i)=HPNRM(1,i);
Get PNRM estimates of response yPNRM(i)=Hat_PNRM*y;
end
degree of freedom=n-sum(a),
PRESS=sum((y-yPNRMcv).∧2),
```

```
SSE=sum((y-yPNRM).^2),
R_squared=100*(1-(SSE/SSM)),
PRESS*=PRESS/(n-sum(a)),
PRESS**=PRESS/((n-sum(a))+(n-k-1)*(SSEmax-SSE)/SSEmax),
%%%%%%%%%% Conditional statement to ensure local bandwidths are all %%%%%%%%%% within (0,1];
if PRESS_DOUBLE_STAR<0;
pdstar=919191919;
elseifmin(b1)<0.0000;
pdstar=7888888888;
elseifmax(b1)>1.0000;
pdstar=522222222;
elseif min(b2)<0.0000;
pdstar=888888888;
elseif max(b2)>1.0000;
pdstar=222222222;
else pdstar=PRESS/((n-sum(a))+(n-k-1)*(SSEmax_LB1-ySSEb)/SSEmax_LB1);
end
press=pdstar;
%%% Display b1, b2,
```

Note: This computer programme is coupled with the genetic algorithm tool in Matlab using my_PNRM_program as fitness function.