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The Adaptive Nonparametric Regression Model and Its Residuals with a Mixing Parameter for Response Surface Methodology: A Novel Blend

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ABSTRACT

The modeling stage of response surface methodology (RSM) includes the application of regression models to estimate the functional relationship between the response and the explanatory variables which demands using data generated from an appropriate 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 tend to underferformed when the homoscedasticity assumption is sullied. In the literature, the use of semiparametric regression models is the preferred techniques in RSM, becauce it combines features of parametric and nonparametric regression models, unlike the nonparametric regression models that are affected by the idiocyncracies of RSM data. In this paper, we consider a novel integration (blend) between an existing adaptive nonparametric regression model and a locally adaptive bandwidths selector generated from the explanatory variables for adequate smoothing of the data. The adaptive nonparametric regression model incorporate local linear regression (LLR) portion and product of the optimal mixing parameter and, the residuals of the LLR to provide a second opportunity of fitting part of the data that were not captured by the LLR model and while the locally adaptive bandwidths addresses the problems associated with dimensionality, sparsity of RSM data and cost efficient design. In the application of RSM data, two data type were considered, and we observed that the goodness-of-fits statistics, zero residual plots, and optimization results of the novel integration (blend) model when compared with the OLS, Model Robust Regression 1(MRR1) and Model Robust Regression 2 (MRR2) considerably performed better.

1. INTRODUCTION

Nair *et al*. (2014) and Yeniay (2014) defined RSM as statistical technique used by engineers and industrial statistician for experimental model building, with the intention of optimizing the response variables which is influenced by several explanatory variables.

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RSM is appropriate for optimizing the response variable $\boldsymbol{y}$ as a function of several explanatory variables $(x_{i1}, x_{i2}, \ldots, x_{ik})$ which is given as:

$$y_i = f(x_{i1}, x_{i2}, \ldots, x_{ik}) + \varepsilon_i, \quad i = 1,2, \ldots, n \tag{1}$$

where ε_i is the error term and assumed to be normally distributed with mean zero and variance $\boldsymbol{\sigma}^2$. The surface as given in (1) characterized by $f(x_{i1}, x_{i2}, \ldots, x_{ik})$ is termed a response surface (Wan and Birch, 2011).

1.2 Ordinary Least Squares (OLS)

The common method for estimating the parameter vector is usually based on the Method of Ordinary Least Squares (OLS). The parameter vector estimates $\widehat{\boldsymbol{\beta}}$ is given as:

$$\widehat{\boldsymbol{\beta}}^{(OLS)} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'y \tag{2}$$

The estimated responses for the i^{th} location can be written as :

$$\hat{y}_i^{(OLS)} = \boldsymbol{x}_i'\widehat{\boldsymbol{\beta}}^{(OLS)} = \boldsymbol{x}_i'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'y, \qquad i = 1,2, \ldots, n \tag{3}$$

where $\boldsymbol{x}_i'$ is the i^{th} row of matrix $\boldsymbol{X}$, $\boldsymbol{X}$ is a matrix with dimension $n \times (k + 1)$.

$\boldsymbol{H}_i = \boldsymbol{x}_i'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'$ is the i^{th} row of the OLS "HAT" matrix of dimension $n \times n$, $\boldsymbol{H}^{(OLS)}$. The estimated response in the i^{th} location is given as:

$$\hat{y}^{(OLS)} = \boldsymbol{H}y\,. \tag{4}$$

where the matrix $\boldsymbol{H}$ is given as:

$$\boldsymbol{H} = \begin{bmatrix} \boldsymbol{H_1} \\ \boldsymbol{H_2} \\ \vdots \\ \boldsymbol{H_n} \end{bmatrix}, \tag{5}$$

(Carley, *et al*., (2004); River (2009))

1.3 MODEL ROBUST REGRESSION 1 (MRR1)

An effective model that addresses the drawbacks inherent in both parametric and nonparametric regression models is the use of semiparametric regression model, Model Robust Regression 1 (MRR1).

The mathematical expression for the MRR1 as given in Einsporn (1987; 1993)as:

$$\hat{y}^{(MRR1)} = \lambda\hat{y}^{(LLR)} + (1 - \lambda)\hat{y}^{(OLS)} \tag{6}$$

where the parameter λ is the mixing parameter with an interval [0, 1].

1.4 MODEL ROBUST REGRESSION 2 (MRR2)

Model Robust Regression 2 (MRR2) combines estimates of parametric regression model to the raw data, while the nonparametric regression model portion, uses the LLR Hat matrix to fit the residuals from the estimates of parametric regression model through a mixing parameter, λ.

The MRR2 was developed by Mays *et al.*, (2001) and is expressed as:

$$\hat{y}^{(MRR2)} = \hat{y}^{(OLS)} + \lambda\hat{r}^{(LLR)}, \quad \hat{r}^{(LLR)} = \boldsymbol{H}_{\boldsymbol{r}}^{(LLR)}r \tag{7}$$

$\lambda \in [0, 1], r = y - y^{OLS}$ is the vector of residuals that represents the structure in the data not captured by the user specified parametric regression model.

1.5 OPTIMIZATION PHASE IN RSM

This involves the use of optimization tools (e.g. Genetic algorithm) in finding the optimal settings of the explanatory variables for which the fitted regression model is optimized. In RSM, two types of optimization problems exist, such as: single response optimization problem and multiple response optimization problems. The last phase of optimization, is to obtain the overall desirability, which is the geometric mean of the individual desirability (Pickle, 2006; He *et al.*, 2012; Adalarasan and Santhanakumar, 2015; Eguasa *et al*., 2022).

1.6 ADAPTIVE NONPARAMETRIC REGRESSION MODEL

In order to address this inadequate utilization of the flexibility of MRR2, we give the existing adaptive nonparametric regression model, PM2 for easy reference.

The mathematical expression of PM2 estimate, $\hat{y}_i^{(PM2)}$ is defined by

$$\hat{y}_i^{(PM2)} = \hat{y}_i^{(LLR)} + \lambda h_i^{(LLR)}[(y_i - \hat{y}_i^{(LLR)})], \qquad i = 1,2, \ldots, n. \tag{8}$$

The PM2 is applied in the estimation of the unknown function f in Equation (1) see Eguasa *et al.* (2019).

1.7 LOCALLY ADAPTIVE BANDWIDTHS SELECTOR

The locally adaptive bandwidths selector includes two aspects of RMS data namely; kth number of explanatory variables in the study and sparseness of the data as given in Eguasa *et al*. (2022) can be expressed mathematically as:

$$b_{ij} = T_{1j}\left(\frac{1}{2} - \frac{x_{ij}}{T_{2j}}\right)^2, \; i = 1,2, \ldots, n; j = 1,2, \ldots, k. \tag{9}$$

where the locally adaptive optimal bandwidths from Equation (9) is obtained at an optimally selected values of T_{1j}, T_{2j}, the tuning parameters (hereafter referred to as T_{1j}^* and T_{2j}^*, respectively), $j = 1,2, \ldots, k$, based on the minimization of the $PRESS^{**}$ criterion.

2. METHODOLOGY

In spite of the flexibility of nonparametric regression methods, they are scantily applied in RSM due to the idiocyncracies of RSM data namely; curse of dimensionality, sparseness of RSM data and cost efficient design. In this paper, we consider a new integration between an existing adaptive nonparametric regression model and a locally adaptive bandwidths selector generated from the explanatory variables, which is embedded in the kernel weight matrix of the adaptive nonparametric regression model. The existing nonparametric regression model incorporate a portion of LLR estimates and product of the optimal mixing parameter and the residuals to provide a second opportunity of fitting part of the data that were not captured by the LLR portion of the model and while the locally adaptive bandwidths addresses the problems associated with dimensionality, sparsity of RSM data and small sample size, see (Eguasa *et al*., 2022).

2.1. INTEGRATING THE ADAPTIVE NONPARAMETRIC REGRESSION MODEL AND LOCALLY ADAPTIVE BANDWIDTHS

In order to address the scanty utilization of the flexibility of MRR2, we concatinate Equations (8) and (9) respectively, a novel blend or approach.

The assumptions of PM2 and locally adaptive bandwidths are given below:

1. $\boldsymbol{x_{ij}} \in [0, 1]$, is a vector of kth explanatory variables at location i, $\forall\, i = 1, 2, \ldots, n; j = 1,2, \ldots, k$.

2. The optimal chosen tuning parameters T_{1j}^{*} , $T_{2j}^{*} > 0$ in all k explanatory variables
3. The optimal mixing parameter $\lambda \in [0, 1]$
4. The optimal chosen bandwidths $b_{ij} \in (0,], \quad \forall\, i = 1, 2, \ldots, n; j = 1,2, \ldots, k$; for smoothing the data at location i and k explanatory variables.

The mathematical expression of PM2 estimate, $\hat{y}_i^{(PM2)}$ is defined by

$$\hat{y}_i^{(PM2)} = \hat{y}_i^{(LLR)} + \lambda h_i^{(LLR)}[(y_i - \hat{y}_i^{(LLR)})], \qquad i = 1,2, \ldots, n. \tag{8}$$

$$b_{ij} = T_{1j}\left(\frac{1}{2} - \frac{x_{ij}}{T_{2j}}\right)^2, \; i = 1,2, \ldots, n; j = 1,2, \ldots, k. \tag{9}$$

The PM2 is applied in the estimation of the unknown function f in Equation (1). As soon as the PM2 and b_{ij} are combined to fit the data, we have a novel blend or approach which is now referred to as ANPM2 for easy referencing.

Hence, the ANPM2 estimate $\hat{y}_i^{(ANPM2)}$ of the response is given as:

$$\hat{\boldsymbol{y}}_{\boldsymbol{i}}^{(ANPM2)} = \boldsymbol{x}_{\boldsymbol{i}}^{\prime(LLR)}\left(\boldsymbol{X}^{\prime(LLR)}\boldsymbol{W}_{\boldsymbol{i}}\boldsymbol{X}^{(LLR)}\right)^{-\mathbf{1}}\boldsymbol{X}^{\prime(LLR)}\boldsymbol{W}_{\boldsymbol{i}}y + \lambda\, \boldsymbol{x}_{\boldsymbol{i}}^{\prime(LLR)}\left(\boldsymbol{X}^{\prime(LLR)}\boldsymbol{W}_{\boldsymbol{i}}^{*}\boldsymbol{X}^{(LLR)}\right)^{-\mathbf{1}}\boldsymbol{X}^{\prime(\boldsymbol{LLR})}\boldsymbol{W}_{\boldsymbol{i}}^{*}\left[y - \boldsymbol{x}_{\boldsymbol{i}}^{\prime(LLR)}\left(\boldsymbol{X}^{\prime(LLR)}\grave{\boldsymbol{W}}_{\boldsymbol{i}}\boldsymbol{X}^{(LLR)}\right)^{-\mathbf{1}}\boldsymbol{X}^{\prime(LLR)}\grave{\boldsymbol{W}}_{\boldsymbol{i}}y\right] \tag{10}$$

where $y = (y_1, \ldots y_n)'$, $\boldsymbol{x}_{\boldsymbol{i}}^{\prime(LLR)} = (1\; x_{i1} \ldots x_{ik})$ is the i^{th} row of the local linear regression model matrix, $\boldsymbol{X}^{(LLR)}$ given as:

$$\boldsymbol{X}^{(LLR)} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix} \tag{11}$$

where the kernel weight matrix is given by

$$\boldsymbol{W}_{\boldsymbol{i}} = \begin{bmatrix} w_{i1} & 0 & \cdots & 0 \\ 0 & w_{i2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w_{in} \end{bmatrix}, i = 1, \; 2\;, \;.\;.\;.\;.\;, n\,. \tag{12}$$

(Wan and Birch, 2011; Eguasa *et al*., 2019).

The kernel function $K\left(\frac{x_{ij}-x_{1j}}{b_{ij}}\right)$ is a simplified Gaussian kernel for one explanatory variable case, given as:

$$w_{i1} = K\left(\frac{x_{ij}-x_{1j}}{b_{ij}}\right) = e^{-\left(\frac{x_{ij}-x_{1j}}{b_{ij}}\right)^2} \tag{13}$$

Otherwise, the kernel function is a product kernel given as:

$$w_{i1} = \prod_{j=1}^{k} K\left(\frac{x_{ij}-x_{1j}}{b_{ij}}\right) \Big/ \sum_{p=1}^{n} \prod_{j=1}^{k} K\left(\frac{x_{pj}-x_{1j}}{b_{ij}}\right), p = 1,2, \dots, n, j = 1,2, \dots, k, \tag{14}$$

For $i = 1$ in Equations (10) and (12), and concantinating the existing bandwidths into the regression model to obtain a novel adaptive regression model . Thus, we have:

$$\hat{\boldsymbol{y}}_{\mathbf{1}}^{(ANPM2)} = \boldsymbol{x}_{\mathbf{1}}^{\prime(LLR)}\left(\boldsymbol{X}^{\prime(LLR)}\boldsymbol{W}_{\mathbf{1}}\boldsymbol{X}^{(LLR)}\right)^{-\mathbf{1}}\boldsymbol{X}^{\prime(LLR)}\boldsymbol{W}_{\mathbf{1}}y + \lambda\, \boldsymbol{x}_{\mathbf{1}}^{\prime(LLR)}\left(\boldsymbol{X}^{\prime(LLR)}\boldsymbol{W}_{\mathbf{1}}^{*}\boldsymbol{X}^{(LLR)}\right)^{-\mathbf{1}}\boldsymbol{X}^{\prime(\boldsymbol{LLR})}\boldsymbol{W}_{\mathbf{1}}^{*}\left[y - \boldsymbol{x}_{\mathbf{1}}^{\prime(LLR)}\left(\boldsymbol{X}^{\prime(LLR)}\grave{\boldsymbol{W}}_{\mathbf{1}}\boldsymbol{X}^{(LLR)}\right)^{-\mathbf{1}}\boldsymbol{X}^{\prime(LLR)}\grave{\boldsymbol{W}}_{\mathbf{1}}y\right] \tag{15}$$

$$\boldsymbol{W}_{\mathbf{1}} = \begin{bmatrix} w_{11} & 0 & \cdots & 0 \\ 0 & w_{12} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w_{1n} \end{bmatrix}_{(n\times n)} \tag{16}$$

The entries from Equation (16) and the locally adaptive bandwidths of Eguasa *et al*. (2022) are translated to estimate $\hat{y}_1^{ANPM2}$**,**

$$w_{11} = \frac{\prod_{j=1}^{k} K\left(\frac{x_{1j}-x_{1j}}{b_{ij}}\right)}{\sum_{p=1}^{n}\prod_{j=1}^{k} K\left(\frac{x_{pj}-x_{1j}}{b_{pj}}\right)}, \quad p = 1, 2, \dots, n; j = 1, 2, \dots, k. \tag{17}$$

$$w_{12} = \frac{\prod_{j=1}^{k} K\left(\frac{x_{2j}-x_{1j}}{b_{ij}}\right)}{\sum_{p=1}^{n}\prod_{j=1}^{k} K\left(\frac{x_{pj}-x_{1j}}{b_{pj}}\right)}, \quad p = 1, 2, \dots, n; j = 1, 2, \dots, k. \tag{18}$$

$$\vdots$$

$$w_{1n} = \frac{\prod_{j=1}^{k} K\left(\frac{x_{nj}-x_{1j}}{b_{ij}}\right)}{\sum_{p=1}^{n}\prod_{j=1}^{k} K\left(\frac{x_{pj}-x_{1j}}{b_{pj}}\right)}, \quad p = 1, 2, \dots, n; j = 1, 2, \dots, k. \tag{19}$$

To estimate, $\hat{y}_2^{ANPM2}$ set $i = 2$ in Equation (10) and (12), we have:

$$\hat{\boldsymbol{y}}_{\boldsymbol{2}}^{(ANPM2)} = \boldsymbol{x}_{\boldsymbol{2}}'^{(LLR)}\left(\boldsymbol{X}'^{(LLR)}\boldsymbol{W}_{\boldsymbol{2}}\boldsymbol{X}^{(LLR)}\right)^{-\boldsymbol{1}}\boldsymbol{X}'^{(LLR)}\boldsymbol{W}_{\boldsymbol{2}}y + \lambda\, \boldsymbol{x}_{\boldsymbol{2}}'^{(LLR)}\left(\boldsymbol{X}'^{(LLR)}\boldsymbol{W}_{\boldsymbol{2}}^{*}\boldsymbol{X}^{(LLR)}\right)^{-\boldsymbol{1}}\boldsymbol{X}'^{(\boldsymbol{LLR})}\boldsymbol{W}_{\boldsymbol{2}}^{*}\left[y - \boldsymbol{x}_{\boldsymbol{2}}'^{(LLR)}\left(\boldsymbol{X}'^{(LLR)}\grave{\boldsymbol{W}}_{\boldsymbol{2}}\boldsymbol{X}^{(LLR)}\right)^{-\boldsymbol{1}}\boldsymbol{X}'^{(LLR)}\grave{\boldsymbol{W}}_{\boldsymbol{2}}y\right] \tag{20}$$

$$\boldsymbol{W}_{\boldsymbol{2}} = \begin{bmatrix} w_{21} & 0 & \cdots & 0 \\ 0 & w_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w_{2n} \end{bmatrix}_{(n\times n)} \tag{21}$$

The entries from Equation (21) and the locally adaptive bandwidths of Eguasa *et al*. (2022) are translated to estimate $\hat{\boldsymbol{y}}_{\boldsymbol{2}}^{\boldsymbol{ANPM2}}$,

$$w_{21} = \frac{\prod_{j=1}^{k} K\left(\frac{x_{1j}-x_{2j}}{b_{ij}}\right)}{\sum_{p=1}^{n}\prod_{j=1}^{k} K\left(\frac{x_{pj}-x_{2j}}{b_{pj}}\right)}, \quad p = 1,\ 2\ ,\ .\ .\ .\ .\ , n; j = 1,\ 2, \dots, k. \tag{22}$$

$$w_{22} = \frac{\prod_{j=1}^{k} K\left(\frac{x_{2j}-x_{2j}}{b_{ij}}\right)}{\sum_{p=1}^{n}\prod_{j=1}^{k} K\left(\frac{x_{pj}-x_{2j}}{b_{pj}}\right)}, \quad p = 1,\ 2\ ,\ .\ .\ .\ .\ , n; j = 1,\ 2, \dots, k. \tag{23}$$

$$w_{2n} = \frac{\prod_{j=1}^{k} K\left(\frac{x_{nj}-x_{2j}}{b_{ij}}\right)}{\sum_{p=1}^{n}\prod_{j=1}^{k} K\left(\frac{x_{pj}-x_{2j}}{b_{pj}}\right)}, \quad p = 1,\ 2\ ,\ .\ .\ .\ .\ , n; j = 1,\ 2, \dots, k. \tag{24}$$

To estimate, $\hat{y}_n^{ANPM2}$ set $i = n$ in Equation (10) and (12), we have:

$$\hat{\boldsymbol{y}}_{\boldsymbol{n}}^{(ANPM2)} = \boldsymbol{x}_{\boldsymbol{n}}'^{(LLR)}\left(\boldsymbol{X}'^{(LLR)}\boldsymbol{W}_{\boldsymbol{n}}\boldsymbol{X}^{(LLR)}\right)^{-\boldsymbol{1}}\boldsymbol{X}'^{(LLR)}\boldsymbol{W}_{\boldsymbol{n}}y + \lambda\, \boldsymbol{x}_{\boldsymbol{n}}'^{(LLR)}\left(\boldsymbol{X}'^{(LLR)}\boldsymbol{W}_{\boldsymbol{n}}^{*}\boldsymbol{X}^{(LLR)}\right)^{-\boldsymbol{1}}\boldsymbol{X}'^{(\boldsymbol{LLR})}\boldsymbol{W}_{\boldsymbol{n}}^{*}\left[y - \boldsymbol{x}_{\boldsymbol{n}}'^{(LLR)}\left(\boldsymbol{X}'^{(LLR)}\grave{\boldsymbol{W}}_{\boldsymbol{n}}\boldsymbol{X}^{(LLR)}\right)^{-\boldsymbol{1}}\boldsymbol{X}'^{(LLR)}\grave{\boldsymbol{W}}_{\boldsymbol{n}}y\right] \tag{25}$$

$$\boldsymbol{W}_{\boldsymbol{n}} = \begin{bmatrix} w_{n1} & 0 & \cdots & 0 \\ 0 & w_{n2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w_{nn} \end{bmatrix}_{(n\times n)} \tag{26}$$

The entries from Equation (26) and the locally adaptive bandwidths of Eguasa *et al*. (2022) are translated to estimate $\hat{\boldsymbol{y}}_{\boldsymbol{n}}^{\boldsymbol{ANPM2}}$,

$$w_{n1} = \frac{\prod_{j=1}^{k} K\left(\frac{x_{1j}-x_{nj}}{b_{ij}}\right)}{\sum_{p=1}^{n}\prod_{j=1}^{k} K\left(\frac{x_{pj}-x_{nj}}{b_{pj}}\right)}, \quad p = 1, \; 2 \;, \; . \; . \; . \; . \;, n; j = 1,\; 2, \dots, k. \tag{27}$$

$$w_{n2} = \frac{\prod_{j=1}^{k} K\left(\frac{x_{2j}-x_{nj}}{b_{ij}}\right)}{\sum_{p=1}^{n}\prod_{j=1}^{k} K\left(\frac{x_{pj}-x_{nj}}{b_{pj}}\right)}, \quad p = 1, \; 2 \;, \; . \; . \; . \; . \;, n; j = 1,\; 2, \dots, k. \tag{28}$$

$$w_{nn} = \frac{\prod_{j=1}^{k} K\left(\frac{x_{nj}-x_{nj}}{b_{ij}}\right)}{\sum_{p=1}^{n}\prod_{j=1}^{k} K\left(\frac{x_{pj}-x_{nj}}{b_{pj}}\right)}, \quad p = 1, \; 2 \;, \; . \; . \; . \; . \;, n; j = 1,\; 2, \dots, k. \tag{29}$$

with respective diagonal matrices of kernel weights, $\boldsymbol{W_2}, \boldsymbol{W_3}, \dots, \boldsymbol{W_n}$ follows pattern from Equations (27, 28 and 29).

Using matrix notation, the ANPM2 can be expressed as:

$$\hat{y}^{(ANPM2)} = \begin{bmatrix} \boldsymbol{h_1^{(LLR)}}y + \boldsymbol{\lambda h_1^{(LLR)}}(y - (\boldsymbol{h_1^{(LLR)}}y) \\ \boldsymbol{h_2^{(LLR)}}y + \boldsymbol{\lambda h_2^{(LLR)}}(y - (\boldsymbol{h_2^{(LLR)}}y) \\ \vdots \\ \boldsymbol{h_n^{(LLR)}}y + \boldsymbol{\lambda h_n^{(LLR)}}(y - (\boldsymbol{h_n^{(LLR)}}y) \end{bmatrix}, \tag{30}$$

$$\hat{y}^{(ANPM2)} = \begin{bmatrix} \boldsymbol{h_1^{(LLR)}} + \boldsymbol{\lambda h_1^{(LLR)}}(\boldsymbol{I} - (\boldsymbol{h_1^{(LLR)}}) \\ \boldsymbol{h_2^{(LLR)}} + \boldsymbol{\lambda h_2^{(LLR)}}(\boldsymbol{I} - (\boldsymbol{h_2^{(LLR)}}) \\ \vdots \\ \boldsymbol{h_n^{(LLR)}} + \boldsymbol{\lambda h_n^{(LLR)}}(\boldsymbol{I} - (\boldsymbol{h_n^{(LLR)}}) \end{bmatrix} y, \tag{31}$$

$$\hat{y}^{(ANPM2)} = \boldsymbol{H}^{(ANPM2)}y \qquad , \tag{32}$$

where $\boldsymbol{I}$ is the $n \times n$ identity matrix, the $1\times n$ vector

$\boldsymbol{h_i^{(LLR)}} + \boldsymbol{\lambda h_i^{(LLR)}}(\boldsymbol{I} - (\boldsymbol{h_i^{(LLR)}})$ is the i^{th} row of the $n \times n$ ANPM2 Hat matrix $\boldsymbol{H}^{(ANPM2)}$.

Using matrix notation, the ANPM2 estimate of the response is given as:

$$\hat{y}^{(ANPM2)} = \begin{bmatrix} \boldsymbol{h}_{\boldsymbol{1}}^{(\boldsymbol{ANPM2})} \\ \boldsymbol{h}_{\boldsymbol{2}}^{(\boldsymbol{ANPM2})} \\ \vdots \\ \boldsymbol{h}_{\boldsymbol{n}}^{(\boldsymbol{ANPM2})} \end{bmatrix} y, \tag{33}$$

$$\hat{y}^{(ANPM2)} = \boldsymbol{H}^{(ANPM2)} y, \tag{34}$$

where $\boldsymbol{h}_{\boldsymbol{i}}^{(\boldsymbol{ANPM2})} = \boldsymbol{h}_{\boldsymbol{i}}^{(LLR)} + \lambda \boldsymbol{h}_{\boldsymbol{i}}^{(LLR)}(\boldsymbol{I} - \boldsymbol{h}_{\boldsymbol{i}}^{(LLR)})$ is the is the i^{th} row of the $n \times n$ ANPM2 Hat matrix $\boldsymbol{H}^{(ANPM2)}$.

2.2. APPLICATION I (SINGLE RESPONSE CHEMICAL PROCESS DATA)

The problem of the study as given in (Pickle *et al.*, 2008) was to relate chemical yield (y) to temperature (x_1) and time (x_2) with the aim to maximize the chemical yield. The data were obtained using the Central Composite Design (CCD) is given in Table 1

Table 1: Single Response Chemical Process Data generated from the Central Composite Design (CCD)

i	x_1	x_2	y
1	-1	-1	88.55
2	1	-1	85.80
3	-1	1	86.29
4	1	1	80.44
5	-1.414	0	85.50
6	1.414	0	85.39
7	0	-1.414	86.22
8	0	1.414	85.70
9	0	0	90.21
10	0	0	90.85
11	0	0	91.31

Source: (Pickle *et al.*, 2008)

2.3. TRANSFORMATION OF DATA FROM CENTRAL COMPOSITE DESIGN (CCD)

In nonparametric regression techniques for RSM, the values of the explanatory variables are designed to lie between 0 and 1. The data collected via a Central Composite Design (CCD) is transformed by a mathematical relation:

$$x_{new} = \frac{Min(x_{old}) - x_0}{(Min(x_{old}) - Max(x_{old}))} \tag{35}$$

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, (Myers *et al*., 2009).

The natural or coded variables in Table 1 are transformed to explanatory variables in Table 2 using Equation (35)

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

$$x_{new} = \frac{Min(x_{old}) - x_0}{\left(Min(x_{old}) - Max(x_{old})\right)}$$

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

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

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

$$x_{new} = \frac{Min(x_{old}) - x_0}{\left(Min(x_{old}) - Max(x_{old})\right)}$$

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

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

Repeating the process up to location 11, then we obtain the entries for explanatory variables x_1 and x_2 respectively in Table 2.

Table 2: The transformed single response chemical process data

i	x_1	x_2	y
1	0.1464	0.1464	88.55
2	0.8536	0.1464	85.80
3	0.1464	0.8536	86.29
4	0.8536	0.8536	80.44
5	0.0000	0.5000	85.50
6	1.0000	0.5000	85.39
7	0.5000	0.0000	86.22
8	0.5000	1.0000	85.70
9	0.5000	0.5000	90.21
10	0.5000	0.5000	90.85
11	0.5000	0.5000	91.31

Source: (Myers *et al*., 2009)

3. RESULTS 1

In single response chemical process data as given in section 3.1, we seek to show the performance of $ANPM2_{PAB}$ over OLS, $MRR1_{PAB}$ and $MRR2_{PAB}$ based on the goodness-of-fit statistics and the process requirements.

The fixed mixing parameters for the models $ANPM2_{PAB}$, $MRR1_{PAB}$ and $MRR2_{PAB}$ as obtained via genetic algorithm tool in MATLAB 7.10.0.499 (R2010a) are presented in Table 3.

Table 3: Mixing Parameters of different models for Single Response Chemical Process Data

Response	**Model**	$\boldsymbol{\lambda}$
y	OLS	NOT APPLICABLE
	$MRR1_{PAB}$	0.9588
	$MRR2_{PAB}$	1.0000
	$ANPM2_{PAB}$	1.0000

Table 4: Comparison of the *goodness-of-fit statistics* of each method for the Chemical Process Data

METHOD	b^*	DF_{error}	MSE	SSE	R^2	R^2_{adj}	$PRESS$	$PRESS^*$	$PRESS^{**}$
OLS	-	5.000	3.1600	15.8182	83.8800	67.7700	109.5179	21.9036	21.9036
$MRR1_{PAB}$	*	2.1751	0.3771	0.8203	99.1644	96.1584	45.6825	21.0028	4.5288
$MRR2_{PAB}$	*	2.0000	**0.3053**	**0.6107**	99.3800	96.8900	43.2389	21.6194	4.4617
$ANPM2_{PAB}$	*	2.0120	0.3094	0.6225	**99.4000**	**97.0000**	**40.7993**	**20.2776**	**4.1006**

In Table 4, $ANPM2_{PAB}$ performed better in terms $PRESS$, $PRESS^*$, $PRESS^{**}$, R^2 and R^2_{adj} statistics, whereas $MRR2_{PAB}$ has the smallest SSE and MSE statistics. "*" represents PAB.

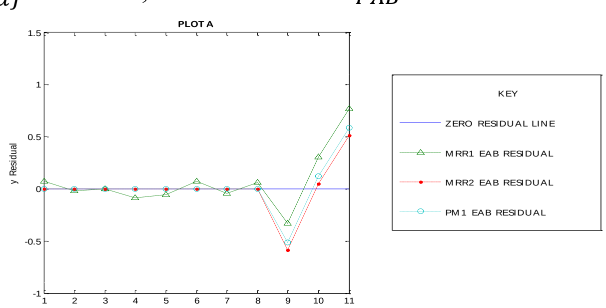

Figure 1: Residual Plot for Single Response Chemical Process Data

Figure 1, is the residual plots for the three models as specified in the KEY for single response chemical process data. Obviously, $MRR2_{PAB}$ estimated the data better in terms of *SSE* and *MSE*. Whereas, $ANPM2_{PAB}$considerably estimated the data in terms of $R^2, R_{adj}^2, PRESS, PRESS*$ $and\ PRESS**$.

Table 5: Comparison of optimization results for the Chemical Process Data

Approach	x_1	x_2	$\hat{y}$
OLS	0.4393	0.4361	90.9783
$MRR1_{PAB}$	0.0007	0.0018	89.2913
$MRR2_{PAB}$	0.2605	0.8009	91.5727
$ANPM2_{PAB}$	$\mathbf{0.7511}$	$\mathbf{0.5101}$	$\mathbf{92.8390}$

The proposed model, $ANPM2_{PAB}$ performs better than existing models in terms of maximum chemical yield for single response chemical process data as given in Table 5. Obviously, $ANPM2_{PAB}$ has a better experimental relationship between temperature (x_1) and time (x_2) as it relates to chemical yield.

3.1. APPLICATION II (MULTI-RESPONSE CHEMICAL PROCESS DATA)

This problem is analyzed in (He *et al*., (2012)). The aim of the study is to get 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 $L = 78.5$, and target value $\emptyset = 80$;

$y_2$should take a value in the range $L = 62$ and $U = 68$ with $\emptyset$ =65;

Minimize $y_3$with upper limit $U = 3300$ and target value $\emptyset = 3100$.

Based on the process requirements a Central Composite Design (CCD) was conducted to establish the design experiment and observed responses as presented in Table 6.

Table 6: Designed experiment and response values for the multi-response chemical process data

i	*Experimental variables*		Responses		
	x_1	x_2	y_1	y_2	y_3
1	-1	-1	76.5	62	2940
2	1	-1	78.0	66	3680
3	-1	1	77.0	60	3470
4	1	1	79.5	59	3890
5	-1.414	0	75.6	71	3020
6	1.414	0	78.4	68	3360
7	0	-1.414	77.0	57	3150
8	0	1.414	78.5	58	3630
9	0	0	79.9	72	3480
10	0	0	80.3	69	3200
11	0	0	80.0	68	3410
12	0	0	79.7	70	3290
13	0	0	79.8	71	3500

Source: He *et al.*, (2012)

The values of the explanatory variables are transformed by the relation in Equation (41) coded between 0 and 1 as given in Table 7.

Table 7: The transformed multiple response chemical process 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

3.2. RESULTS 2

In the multiple response chemical process data as given in section 3.4, we seek to show the performance of $ANPM2_{PAB}$ over OLS, $MRR1_{PAB}$ and $MRR2_{PAB}$ based on the goodness-of-fit statistics and the process requirements.

The fixed mixing parameters for the models, $ANPM2_{PAB}$, $MRR1_{PAB}$ and $MRR2_{PAB}$, as obtained via genetic algorithm tool in MATLAB 7.10.0.499 (R2010a) are presented in Table 8.

Table 8: Mixing Parameters of different models for Multiple Chemical Process Data

Response	**Model**	$\boldsymbol{\lambda}$
y_1	OLS	NOT APPLICABLE
	$MRR1_{PAB}$	1.0000
	$MRR2_{PAB}$	1.0000
	$ANPM2_{PAB}$	1.0000
y_2	OLS	NOT APPLICABLE
	$MRR1_{PAB}$	0.7085
	$MRR2_{PAB}$	1.0000
	$ANPM2_{PAB}$	0.9433
y_3	OLS	NOT APPLICABLE
	$MRR1_{PAB}$	0.9320
	$MRR2_{PAB}$	1.0000
	$ANPM2_{PAB}$	0.6999

Table 9: Model *goodness-of-fit statistics* for Multiple Chemical Process Data

Response	**Model**	$\boldsymbol{DF}$	$\boldsymbol{PRESS^{**}}$	$\boldsymbol{PRESS}$	$\boldsymbol{SSE}$	$\boldsymbol{MSE}$	$\boldsymbol{R^2}$**(%)**	$\boldsymbol{R^2_{Adj}}$**(%)**
y_1	OLS	7.0000	-	-	0.4962	0.4962	98.2733	97.0400
	$MRR1_{PAB}$	4.0144	0.0481	0.6687	0.2165	0.0539	99.2469	97.7489
	$MRR2_{PAB}$		0.0984	0.9548	**0.2131**	**0.0533**	**99.2600**	**97.7800**
	$ANPM2_{PAB}$	4.0121	**0.0480**	**0.6675**	0.2151	0.0536	99.2515	97.7613
y_2	OLS	7.0000	-	-	36.2242	5.1749	89.9725	82.8100
	$MRR1_{PAB}$	4.8751	7.5752	107.9471	12.2280	2.5083	96.6149	91.6676
	$MRR2_{PAB}$	4.0000	9.7470	109.5441	**10.0023**	2.5006	97.2300	91.6900
	$ANPM2_{PAB}$	4.0714	**4.7577**	**65.6015**	10.0051	**2.4574**	**97.2303**	**91.8365**
y_3	OLS	7.0000	-	-	207870	29696	75.8967	58.6800
	$MRR1_{PAB}$	6.5922	26522	361000	79164	**12009**	90.8216	**83.2923**
	$MRR2_{PAB}$	4.0000	50382	545270	66047	16512	92.3400	77.0300
	$ANPM2_{PAB}$	4.0002	**23776**	**275910**	**65720**	16429	**92.3804**	77.1423

In Table 9, $ANPM2_{PAB}$, outperformed OLS, $MRR1_{PAB}$ and $MRR2_{PAB}$ in terms of $PRESS$ and $PRESS^{**}$ with respect to chemical yield (y_1). Whereas, $MRR2_{PAB}$ performed better than other models considered in terms of SSE, MSE, R^2 and R^2_{Adj} for chemical yield (y_1). For viscosity (y_2), $ANPM2_{PAB}$ performed better between than OLS, $MRR1_{PAB}$ and $MRR2_{PAB}$ in terms of PRESS, PRESS**, MSE, R^2 and R^2_{Adj} statistics, while $MRR2_{PAB}$ outperformed OLS, $MRR1_{PAB}$ and $ANPM2_{PAB}$ in terms of SSE.

In terms of molecular weight (y_3), $ANPM2_{PAB}$ outperformed *OLS*, $MRR1_{PAB}$ and $MRR2_{PAB}$ with respect to *PRESS, PRESS**, SSE* and R^2 statistics. $MRR1_{PAB}$ performed better in terms of $MSE\ and\ R^2_{Adj}$.

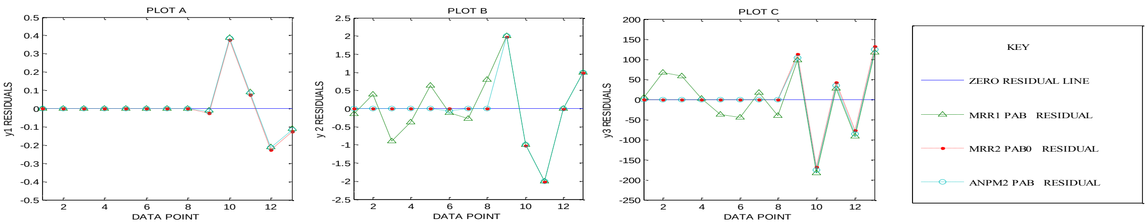

Figure 2. Plot A: maximize chemical yield; Plot B: is a two sided transformation of viscosity; Plot C: minimize molecular weight

$ANPM2_{PAB}$ in the overall performance turns out better in terms of *goodness-of-fit statistics*.

Figure 2 is basically the residual plots for different models as given in the KEY for which the proposed model $ANPM2_{PAB}$ on the average perform better in terms of minimum residual points, meaning $ANPM2_{PAB}$ estimated the data better than other models considered.

Table 10: Model optimal solution based on the Desirability function for multiple 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	3229.9000	0.1744	0.5058	0.3504	31.3800
$MRR1_{PAB}$	0.5458	0.1464	79.3568	64.7911	3196.8000	0.5712	0.9304	0.5162	64.9758
$MRR2_{PAB}$	0.5360	0.2296	78.7880	66.4283	3193.7000	0.1920	0.5239	0.5314	37.6723
$PM2_{PAB}$	**0.0736**	**0.7282**	81.7956	65.0000	3002.5000	1.0000	1.0000	1.0000	**100.0000**

In Table 10, the proposed model $ANPM2_{PAB}$ satisfies the choice of process requirements for a multiple chemical process data. Hence, the overall desirability with the highest percentage gives the best production requirements.

4. DISCUSSION OF RESULTS

In this paper, we have shown a novel blend between locally adaptive bandwidth that is driven by local variability in the data and the adaptive nonparametric regression model for RSM data.

We have compared results of the adaptive nonparametric regression model ($ANPM2_{PAB}$) with OLS, $MRR1_{PAB}$ and $MRR2_{PAB}$ using the same data sets in section 3.1 to 3.5. The $ANPM1_{PAB}$ for single response chemical process data performed better in terms of goodness-of-fit statistics and optimization result over OLS, $MRR1_{PAB}$

and $MRR2_{PAB}$. Though, the multi-response problem, $ANPM2_{PAB}$ performed better than OLS, $MRR1_{PAB}$ and $MRR2_{PAB}$ with respect to goodness-of-fit statistics and the process requirements for the data considered. Furthermore, the locally adaptive bandwidth enhanced the performance of $MRR1_{PAB}$, $MRR2_{PAB}$ and $ANPM2_{PAB}$ in terms of goodness-of-fit statistics for the two data types examined.

5. CONCLUSIONS

In addition, the model $ANPM2_{PAB}$ compared with OLS, $MRR1_{PAB}$ and $MRR2_{PAB}$ performed satisfactorily in terms of goodness-of-fit tests. The model $ANPM2_{PAB}$, again on the average performance did better than existing models $MRR1_{PAB}$ and $MRR2_{PAB}$ in terms of goodness-of-fits statistics and process requirements.

Evidently, the model $ANPM2_{PAB}$ appear to have better performance over the models, $MRR1_{PAB}$ and $MRR2_{PAB}$ in all the RSM data considered in this paper. Conclusively, the adaptive nonparametric regression model incorporate local linear regression (LLR) portion and product of the optimal mixing parameter and, the residuals of the LLR to provide a second opportunity of fitting part of the data that were not captured by the LLR model and while the locally adaptive bandwidths perform adequate smoothing of the three datasets by location for kth number of explanatory variables and as provides a better estimates for the two datasets utilized in this paper.

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DISCLOSURE STATEMENT

No potential conflict of interest was reported by the author(s).

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