

## **Original Research Article**

### **Use of one-factor design of experiments (DOE) for Regression Modelling and Validation: A Robust Methodology**

**Running Title: One-factor design of experiments (DOE) for Regression Modelling**

#### **Abstract:**

In the present research era, high accuracy methods as a statistical analysis tool are increasing. Therefore, researchers are more focused to produce reliable and accurate results. Hence, the use of data modelling techniques is more focused to meet the needs of the current research trend. On the other hand, Design of Experiment (DOE) is extensively used among various scientific fields; however, its limitations do not allow these study designs for modelling purposes. Therefore, this study was designed to develop a methodology combining statistical methods that can provide to use one-factor DOE study designs for modelling and predictions. The addition of Fuzzy regression and multilayer feedforward (MLFF) neural network along with multiple linear regression would provide more accurate results with high accuracy. Furthermore, the developed methodology was tested on a dataset to test the methodology's performance and results provided that methodology provided regression models through MLR and fuzzy with high accuracy with the testing of the model's predictability through MLFF.

#### **Keywords:**

Design of experiment, Regression, Methodology, Robust, MLFF

#### **Introduction:**

DOE study designs are widely used among various scientific and non-scientific experiments and can be used to explore or study the relationship or association among the variables [1-3]. However, the use of DOE study designs is limited to studying the association between the variables and cannot be used for prediction purposes [4]. On the other hand, forecasting is becoming popular and shared in the studies as it helps to improve the significance of the study findings and impact of the research; hence the use of regression modelling has become increasing among the scientific community.

Due to the DOE limitations, these study designs cannot be used for regression modelling. Hence, some prior work, which is called data transformation, is required to use DOE study designs for regression modelling [5]. Furthermore, due to the nature of the independent variables in the DOE study designs, called factors, it is likely to have fuzziness in the transformed data. On the other hand, linear regression models are designed to model crisp datasets, and their aptness becomes poor in case of vague data [6]. Therefore, to address the issue of data fuzziness and incorporate fuzzy data into the regression model, a new approach in regression modelling was introduced, which is called Fuzzy linear regression modelling [7]. Like linear regression, which is based on probability theory, fuzzy regression is based on the theory of possibility [8,9]. L.A. Zadeh did the initial work on fuzzy regression, which later proceeded by Tanaka, Diamond, Ishibuchi and others [8,10,11].

Therefore, this study was designed to provide a methodology that can enable researchers to use their DOE study designs for prediction purposes. The study aim was to provide a comprehensive and robust methodology that included the transformation of one-factor DOE study design to linear form, use of bootstrapping to enhance the accuracy of estimated regression parameters, use of linear and fuzzy regression models and utilization of multilayer feedforwarding (MLFF) neural networking for model validation.

### Methodology:

One factor DOE study design was used for transformation into linear form, followed by regression modelling and validation. Therefore, the data transformation process on generalized one-factor DOE study design was initially elaborated. Hence, Table 1 introduced the distribution of one-factor DOE with  $i$  treatments and  $j$  observations within each treatment.

Table 1: General data distribution for one-factor study design

1	2	Treatment	
		...	i
$y_{11}$	$y_{21}$	...	$y_{i1}$
$y_{12}$	$y_{22}$	...	$y_{i2}$
$y_{13}$	$y_{23}$	...	$y_{i3}$
.	.	...	.
.	.	...	.
.	.	...	.
$y_{1j}$	$y_{2j}$	...	$y_{ij}$

Data presented in table 3.1 has one dependent variable ( $y$ ) and " $i$ " treatments (factors). However, to transform the data into the linear form, " $i^{\text{th}}$ " treatment or factor is not required,

as expressed in terms of  $i-1$  treatments or factors [12]. Therefore, a generalized matrix for the transformed dataset contained  $r=i-1$  and  $n=j$ . Now the utmost part of the transformation process is to code the factor. The variables generated after the coding are called indicator variables that take on values 0, 1 or -1 [5]. This coding process must be done carefully because it leads to the regression coefficients in the  $\beta$  vector. Hence, the matrix obtained after the transformation of the dataset has dependent and independent variables matrix, matrix for slopes and matrix for random error.

$$Y = \begin{bmatrix} Y_{11} \\ Y_{12} \\ \vdots \\ Y_{1n} \\ Y_{21} \\ Y_{22} \\ \vdots \\ Y_{in} \end{bmatrix}; X = \begin{bmatrix} 1 & 1 & 0 & \cdot & 0 \\ 1 & 1 & 0 & \cdot & 0 \\ 1 & 1 & 0 & \cdot & 0 \\ 1 & 1 & 0 & \cdot & 0 \\ 1 & 1 & 0 & \cdot & 0 \\ 1 & 0 & 1 & \cdot & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & -1 & -1 & \cdot & -1 \end{bmatrix}; \beta = \begin{bmatrix} \mu. \equiv \beta_0 \\ \tau_1 = \beta_1 \\ \tau_2 = \beta_2 \\ \tau_3 = \beta_3 \\ \vdots \\ \tau_{i-1} = \beta_{i-1} \end{bmatrix}; \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{12} \\ \vdots \\ \varepsilon_{1n} \\ \varepsilon_{21} \\ \varepsilon_{22} \\ \vdots \\ \varepsilon_{in} \end{bmatrix}$$

Let  $X_{ij1}$  denote the value of indicator variable  $X_1$ ,  $X_{ij2}$  indicate the value of indicator variable  $X_2$ , and so on. Using  $i-1$  indicators in the model and multiple linear regression model can be stated as

$$Y_{ij} = \mu. + \tau_1 x_{ij1} + \tau_2 x_{ij2} + \cdots + \tau_{i-1} x_{ij(i-1)} + \varepsilon_{ij}$$

where,

$$x_{ij1} = \begin{cases} 1 & \text{if the case from the factor level1} \\ -1 & \text{if the case from the factor level(i)} \\ 0 & \text{Otherwise} \end{cases}$$

$$x_{ij2} = \begin{cases} 1 & \text{if the case from the factor level2} \\ -1 & \text{if the case from the factor level(i)} \\ 0 & \text{Otherwise} \end{cases}$$

$$x_{ij(i-1)} = \begin{cases} 1 & \text{if the case from the factor level (i - 1)} \\ -1 & \text{if the case from the factor level (i)} \\ 0 & \text{Otherwise} \end{cases}$$

Therefore, to apply the above process of data transformation to get the linear form, a one-factor DOE data was extracted from a book "Probability & Statistics for Engineers & Scientists" by Walpole R.E et al. The dataset consisted of 25 patients with a fever of 38 degrees Celsius or higher and used five different brands of headache relief medications. The number of hours of headache relief was recorded in Table 2.

Table 2: Hours of relief from five different brands of headache tablets

Group 1	Group 2	Group 3	Group 4	Group 5
5.2	9.1	3.2	2.4	7.1
4.7	7.1	5.8	3.4	6.6
8.1	8.2	2.2	4.1	9.3
6.2	6.0	3.1	1.0	4.2
3.0	9.1	7.2	4.0	7.6

After that, the transformation process was initiated; data in Table 2 had five groups ( $r = 5$ ) and five observations in each group ( $n = 5$ ). Hence, each column of the transformed matrix had 25 observations ( $r \times n$ ). The independent variables' matrix required indicator variables with values ranging from 0, 1 and -1. Therefore, the matrix after transformation looked like this:

$$Y = \begin{bmatrix} Y_{11} \\ Y_{12} \\ Y_{13} \\ Y_{14} \\ Y_{15} \\ Y_{21} \\ \vdots \\ Y_{55} \end{bmatrix}; X = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & -1 & -1 & -1 & -1 \end{bmatrix}; \beta = \begin{bmatrix} \mu. \equiv \beta_0 \\ \tau_1 = \beta_1 \\ \tau_2 = \beta_2 \\ \tau_3 = \beta_3 \\ \tau_4 = \beta_4 \end{bmatrix}; \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{12} \\ \varepsilon_{13} \\ \varepsilon_{14} \\ \varepsilon_{15} \\ \varepsilon_{21} \\ \vdots \\ \varepsilon_{55} \end{bmatrix}$$

Let  $X_{i1}$  denoted the value of indicator variable  $X_1$ ,  $X_{i2}$  indicated the value of indicator variable  $X_2$ , etc. Using  $t-1$  indicators in the model and multiple linear regression model for the study would be stated as

$$Y_i = \mu. + \tau_1 x_{i1} + \tau_2 x_{i2} + \tau_3 x_{i3} + \tau_4 x_{i4} + \varepsilon_i$$

where

$$\begin{aligned} x_{i1} &= \begin{cases} 1 & \text{if the case from the factor level 1} \\ -1 & \text{if the case from the factor level 5} \\ 0 & \text{Otherwise} \end{cases} & x_{i2} &= \begin{cases} 1 & \text{if the case from the factor level 2} \\ -1 & \text{if the case from the factor level 5} \\ 0 & \text{Otherwise} \end{cases} \\ x_{i3} &= \begin{cases} 1 & \text{if the case from the factor level 3} \\ -1 & \text{if the case from the factor level 5} \\ 0 & \text{Otherwise} \end{cases} & x_{i4} &= \begin{cases} 1 & \text{if the case from the factor level 4} \\ -1 & \text{if the case from the factor level 5} \\ 0 & \text{Otherwise} \end{cases} \end{aligned}$$

Table 3 represents the data after transformation. The data had one dependent variable  $Y_{ij}$ , and four  $X_{i1}$ ,  $X_{i2}$ ,  $X_{i3}$ , and  $X_{i4}$ . Data now transformed to linear form and could be used for regression modelling.

$Y_{ij}$	$X_{i1}$	$X_{i2}$	$X_{i3}$	$X_{i4}$
5.2	1	0	0	0
4.7	1	0	0	0
8.1	1	0	0	0
6.2	1	0	0	0
3.0	1	0	0	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
4.2	-1	-1	-1	-1
7.6	-1	-1	-1	-1

```
y = c(5.2, 4.7, 8.1, 6.2, 3.0, 9.1, 7.1, 8.2, 6.0, 9.1, 3.2, 5.8, 2.2, 3.1,  
      7.2, 2.4, 3.4, 4.1, 1.0, 4.0, 7.1, 6.6, 9.3, 4.2, 7.6)  
x1 = c(1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1,  
      -1, -1, -1, -1)  
x2 = c(0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1,  
      -1, -1, -1, -1)  
x3 = c(0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 0, 0, 0, -1,  
      -1, -1, -1, -1)  
x4 = c(0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, -1,
```

-1, -1, -1, -1)

```
X = cbind(x1,x2,x3,x4)
data = data.frame(y,x1,x2,x3,x4)
```

### ***R Syntax for data entry and Bootstrapping***

#### **#/Performing Bootstrap for 1000**

```
mydata <- rbind.data.frame(data, stringsAsFactors = FALSE)
iboot <- sample(1:nrow(mydata),size=1000, replace = TRUE)
bootdata <- mydata[iboot,]
```

### ***R Syntax for splitting bootied data into test and train data***

#### **#/Randomly split the data into 70:30**

#### **#70 percent of the data at our disposal to train the network**

#### **#30 percent to test the network/**

```
smp_size <- floor(0.70*nrow(bootdata))
set.seed(123)
train_ind<- sample(seq_len(nrow(bootdata)), size=smp_size)
```

```
train <- data.frame(bootdata[train_ind,])
test <- data.frame(bootdata[-train_ind,])
```

#### **# Print Data**

```
print(train)
print(test)
```

### ***R Syntax for MLR Regression Modelling***

#### **# /Fit a Linear Regression Model**

#### **# Use Mean Squared Error (MSE) as a Measure of Prediction Performance/**

#### **#/Predict the Values for the Test Set and Calculate the MSE/**

```
Model <- lm(y~x1+x2+x3+x4, data=train)
summary(Model)
predict_lm <- predict(Model,test)
MSE.lm <- sum((predict_lm - test$y)^2)/nrow(test)
```

MSE.lm

### ***Syntax for Fuzzy regression Modelling***

```
if(!require(fuzzyreg)) install.packages("fuzzyreg", dependencies = TRUE)
library(fuzzyreg)
```

#### **##Fuzzy linear model using the PLRLS method##**

```
f <-fuzzylm(y ~ x1+x2+x3+x4, data=train$lee, method = "plrsls", fuzzy.left.x =
NULL, fuzzy.right.x = NULL, fuzzy.left.y = NULL, fuzzy.right.y = NULL)
coef(f)
```

### ***R Syntax for data normalization and Multilayer Feedforward Neural Network***

#### ***#/Performing neural network***

##### ***#/install the neuralnet package/***

```
if(!require(neuralnet)){install.packages("neuralnet")}
library("neuralnet")
```

##### ***#/Scaling the data for normalization***

##### ***# Method (usually called feature scaling) to get all the scaled data***

##### ***# in the range [0,1]/***

```
max_data <- apply(bootdata, 2, max)
min_data <- apply(bootdata, 2, min)
data_scaled <- scale(bootdata,center = min_data, scale = max_data - min_data)
```

##### ***#/Randomly split the data into 70:30***

##### ***#70 percent of the data at our disposal to train the network***

##### ***#30 percent to test the network/***

```
index = sample(1:nrow(bootdata),round(0.70*nrow(bootdata)))
train_data <- as.data.frame(data_scaled[-index,])
test_data <- as.data.frame(data_scaled[-index,])
```

##### ***#/Build the network***

##### ***#Create 2 hidden layers have 3 and 2 neurons respectfully***

##### ***#Input layer = 4***

##### ***#Output layer = 1/***

```
n = names(bootdata)
f = as.formula(paste("y ~", paste(n[!n %in% "y"], collapse = " + ")))
nn = neuralnet(f,data=train_data,hidden=c(3,2),linear.output=T)
plot(nn)
```

```
options(warn=-1)
```

```
#/30 percent of the available data to do this:
```

```
#using only the first 2 columns representing the input variables
```

```
#of the network and 1 is the output for NN/
```

```
predicted <- compute(nn,test_data[,1:4])
```

```
#/Use the Mean Squared Error NN (MSE-forecasts the network) as a measure  
of how far away our predictions are from the real data/
```

```
MSE.net <- sum((test_data$y - predicted$net.result)^2)/nrow(test_data)
```

```
MSE.net
```

```
#/Printing the Value of MSE for Linear Model and Neural Network/
```

```
print(paste(MSE.lm,MSE.net))
```

## Results:

The outcome generated from data after running the R syntax were summarized in this section. Parameters for multiple linear regression were calculated first with the summary of the model. Table 4 summarizes the output for the MLR estimated parameters. Slopes for the parameters  $x_2$ ,  $x_3$  and  $x_4$  were statistically significant ( $p < 0.001$ ).

Table 4: Parameter Estimates of Regression Modelling

Variable	Parameter Estimates		t-value	P-value
	Parameter Estimate	Standard Error		
Intercept	5.56	0.15	35.87	<.0001
$x_1$	-0.104	0.315	-0.329	0.235
$x_2$	2.55	0.306	8.304	<.0001
$x_3$	-2.43	0.325	-7.473	<.0001
$x_4$	-2.03	0.325	-6.244	<.0001

Hence, a multiple linear regression model with estimated parameters can be written as

$$\text{Hours of relief} = 5.56 - 0.104 x_1 + 2.55 x_2 - 2.43 x_3 - 2.03 x_4$$

The model was statistically significant ( $P < 0.0001$ ), and the adjusted R-square was 0.71 (Table 5). To determine the predictability of the MLR model, the MSE (mean square error) of the model was computed, and it was found to be 1.05 (Table 5).

Table 5: MLR Model Summary



Residual SE	1.279	R-Square	0.727
MSE	1.05	Adj R-Sq	0.71
F-statistic	43.36	P-value	<0.0001

Similarly, table 6 tabulated the parameters obtained for fuzzy regression, containing Central, lower and upper boundary values for intercept and variables.

Table 6: Parameter Estimates of Fuzzy Modelling

Variable	Parameter Estimates		
	Central Tendency	Lower Boundary	Upper Boundary
Intercept	5.51	3.68	6.78
x1	-0.007	-0.68	1.32
x2	2.32	2.32	2.32
x3	-1.15	-1.48	0.42
x4	-2.68	-2.68	-2.68

To draw the fuzzy regression equation, a central tendency column was used. However, lower and upper boundary columns were used from table 6 to construct the equation for lower and upper boundaries for boundaries of fuzzy regression. Therefore, the fuzzy regression equations are as follow :

Central tendency of the fuzzy regression model:

$$\text{Hours of relief} = 5.51 - 0.007x_1 + 2.32x_2 - 1.15x_3 - 2.68x_4$$

Lower boundary of the model support interval:

$$\text{Hours of relief} = 3.68 - 0.6845x_1 + 2.32x_2 - 1.48x_3 - 2.68x_4$$

Upper boundary of the model support interval:

$$\text{Hours of relief} = 6.78 + 1.32x_1 + 2.32x_2 + 0.42x_3 - 2.68x_4$$

To quantify that how close the predicted values of the dependent variable (Y) through each model (MLR and Fuzzy), the equations derived above, from MLR and fuzzy, were used on test data to calculate values for predicted Y (Table 7). Furthermore, the absolute difference between original and predicted Y from each model was computed to calculate the numeric difference between original and predicted values of the dependent variable through each model. Therefore, the mean of the absolute difference between MLR and fuzzy was very small; however, fuzzy was marginally better than MLR.

Table 7: Predicted values of Y form MLR and fuzzy models

Y	Predicted Y		Abs difference	
	MLR	Fuzzy	MLR	Fuzzy
9.1	7.5791	7.027	1.5209	2.073
4.2	3.128	4.36	1.072	0.16
6.6	3.528	2.83	3.072	3.77
7.1	7.5791	7.027	0.4791	0.073
6.6	3.528	2.83	3.072	3.77
.	.	.	.	.
.	.	.	.	.
5.8	8.1089	7.83	2.3089	2.03
9.1	8.1089	7.83	0.9911	1.27
8.1	7.5791	7.027	0.5209	1.073
<b>Average</b>			<b>2.16</b>	<b>2.01</b>

MLFF neural network was embedded in the syntax to test the strength of the parameters used in the regression model; therefore, it helped determine how good the forecasting was through the derived regression model. Figure 1 presents the architecture of the neural network obtained from the data. The figure had hidden layers with 3 and 2 neurons, respectively, and as the networking was Feedforward, the information was only carried in the forward direction (figure 1). Furthermore, the calculated MSE for the network was 0.09. Therefore, the minimal error measurement demonstrated that constructed model's accuracy and forecasting capability. As a result, all four independent variables were good predictors of hours of headache relief after taking medicine.

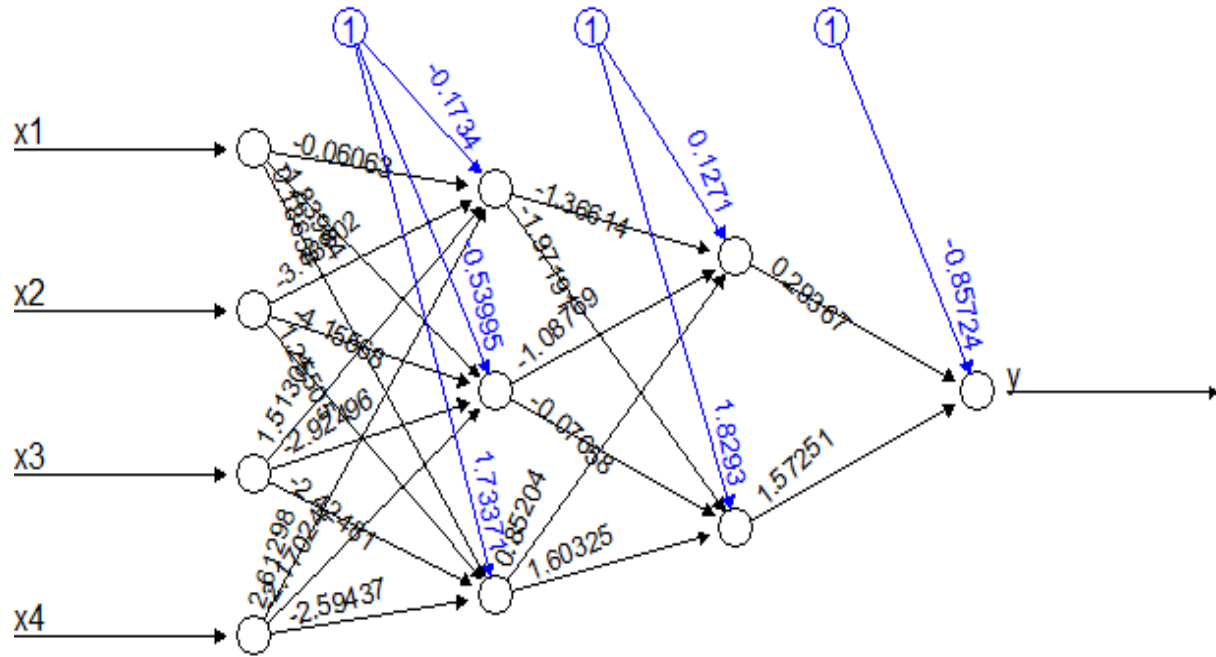


Figure 1: The architecture of the MLFF neural network with four input variables, two hidden layers and one output node

### Conclusion:

This study provided a combined, comprehensive and robust methodology for using one-factor DOE for prediction purposes by transforming DOE into a linear form. Using an independent dataset "test data" to find the predictability of MLR by calculating MSE provided the precision and predictability of the derived model. In addition, this methodology also embedded the fuzzy regression to enhance the predictability and accuracy of the model in case of fuzziness in the data and model performance was evaluated (Table 7) and found estimation from fuzzy was comparatively better. Furthermore, small MSE from the neural network provided that predictions or estimates drawn from the obtained regression model would be very close to actual population characteristics. Therefore, this methodology can allow the research community and academicians to use their DOE study designs for prediction purposes to meet the growing needs of research trends and help them get more improved outcomes from their research.

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$y_{13}$	$y_{23}$	...		$y_{i3}$
.	.	...		.
.	.			.
.	.			.
$y_{1j}$	$y_{2j}$	...		$y_{ij}$

Table 2: Hours of relief from five different brands of headache tablets

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4.7	7.1	5.8	3.4	6.6
8.1	8.2	2.2	4.1	9.3
6.2	6.0	3.1	1.0	4.2
3.0	9.1	7.2	4.0	7.6

Table 3: Regression approach to one-factor DOE

$Y_{ij}$	$X_{i1}$	$X_{i2}$	$X_{i3}$	$X_{i4}$
5.2	1	0	0	0
4.7	1	0	0	0
8.1	1	0	0	0
6.2	1	0	0	0
3.0	1	0	0	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
4.2	-1	-1	-1	-1
7.6	-1	-1	-1	-1

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Figure 1: The architecture of the MLFF neural network with four input variables, two hidden layers and one output node

