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On the Prediction of the Copper Content in the Slag, a Case of Multiple Linear Regression Model, MLR (p)

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Abstract

This paper presented the use of Multiple Linear Regression Analysis (MLRA) in the statistical modeling of the technological processes such as the pyrometallurgical processes for copper extraction. However, this work, out of the six formulated models from the full model and itself, choose the best performed model, hence arranging them in their order of preference; model performances, considering their R-Squared values (R^2), Standard deviation values (std), Variance Information Factor (VIF), Cross-Validated (R^2), Q^2 and the p-values $(sig.values)$. The order of contribution to the model fit of the independent variables of the each formulated model was equally accounted for in this study where the influences of the explanatory variables ($X_{i's}$) on the explained value (Y_i) were evaluated. The result indicated that the order of model performance selection judging with its R-Squared (R^2) and $Std.Dev.$ (S_Y^2) ranged the models from model four, six, full model, one, five, three, and two, whereas assessment of the model performance for the presence of multicollinearity(MC) resulted in selection of the models as follows: model two, three, five, one, full model, six and four, where their Tolerance index values and Variance information factor values were within the acceptance limits according [1]. Finally predictive power of the formulated models which were assessed by their Cross-Validated (R^2), denoted by Q^2, selected these models based on their order of model predictive powers; model four, six, full model, one, five, three, two.

Keywords: *Multiple linear regression, Tolerance index (TI), Copper contents in the slag, Model performances, Predictive error sum of squares, Variance Information Factor(VIF).*

1. Introduction

In the statistical modeling of the technological processes where the influences of the explanatory variables ($X_{i's}$) on the explained value (Y_i) is to be evaluated, Multiple Linear Regression Analysis (MLRA) and the Nonlinear Regression Analysis (NRA) are most often applied, [2]. According to the obtained analytical models, with the certain probability, the $X_{i's}$ values could be used for managing and control of the Y_i value. In the case of complex technical technological processes which copper contents evolution in slag is one of, R^2 of such models is relatively small, resulting with unreliable prediction of the output values. At the same time, if there is more than one output value as of multivariate model, both MRA and the NRA are resulting with limited possibilities of use ([3]; [4]; [5]).

Multiple Linear Regression has been applied extensively as predictive models for engineering and non-engineering domains ([6]; [7]; [8]). [9] used Multiple Linear Regression model to establish an interrelationship among price, recovery and profitability. [10] studied on a Linear Regression Model with power distributions. Moreover several authors like ([11], [12], [13], [14], [1], [15], [16], [17], [18], [19], [20], [21], [22], [23], [24], [25], etc.) have worked with multiple linear regression models.
However, the main aim of this research is to, out of the six formulated models from the full model and itself, chooses the best performed model, hence arranging them in their other of preference; model performances, considering their R-Squared values (R^2), Standard deviation values (std),

Variance Information Factor (VIF),Tolerance Index (TI), cross-validated R^2, Q^2 and the p-values $(sig.values)$. The order of contribution to the model fit of each of the independent variables of the each model formulated was equally accounted for in this study from their fitted equation.

2. Material and Methods

In the pyrometallurgical processes for copper extraction, the essential phase of the operation is smelting operation which produces two results: waste slag, {Cu $_{(slag)}$} and the copper matte, {Cu $_{(matte)}$}. The copper matte is further processed during the complex technological process of copper extraction [26]. Notwithstanding the current phase in the stages of the technology applied [27], for the worldwide problems of the slag deposition, local solutions should be seek out [28]. The dependence of the copper slag on the other copper wastes was tackled analytically with the aid of Multiple Linear Regression Analysis method. Moreover, the data used for this study were secondary data adopted from [29], where this Multiple Linear Regression model applied:

$$y_i = f\left(X_j, \beta\right) + \varepsilon_i \;;\; i = 1, 2, \dots, p \qquad \dots 1$$

p stands for the number of total observation, which is $i = 1, 2, \dots, 67$ and
$X_j = \left(x_{1i}, x_{2i}, \dots, x_{ki} = S_iO_2,\ \text{FeO},\ Fe_3O_4,\ \text{CaO},\ Al_2O_3,\ \text{Cu}_{(matte)}\right)$
is the vector of the concentration of the components in wt. (%), related to y_j $\{Cu_{(slag)}\}$. $\beta = \left(\beta_0, \beta_1, \dots, \beta_p = |\text{a, b, c, d, e, f and g}\right)$ are coefficients of the linear regression equation in equation … (1) and ε_i is the stochastic or random error associated with the ith observation, reorganizing all the usual assumptions according to [30]. This Multiple Linear Regression model could equally be written expressively as

[Cu$_{\{slag\}}$] = a + b (S_iO_2) + c (FeO) + d (Fe_3O_4) + e (CaO) + f (Al_2O_3) + g [Cu$_{\{matte\}}$]

Where: a, b, c, d, e, f and g are coefficients of the linear regression equation, this implies that;

x_1 = the concentration composition of silicon dioxide, (S_iO_2) in percentage x_2 = the concentration composition of iron dioxide, (FeO) in percentage x_3 = the concentration composition of iron tetra oxide, (Fe_3O_4) in percentage x_4 = the concentration composition of calcium dioxide, (CaO) in percentage x_5 = the concentration composition of aluminum II oxide,(Al_2O_3) in percentage x_6 = the concentration of copper matte, g [Cu$_{\{matte\}}$] in percentage y = the concentration composition response of copper slag,[Cu$_{\{slag\}}$] in percentage.

The data sets which were analyzed by the aid of statistical software, IBM SPSS statistics 20 considered stepwise regression selection in order to identify those concentration compositions in wt (%) of the independent variables X that have more significant influence to the response variable y in each of the developed Multiple Linear Regression Models. The formulated Multiple Linear Regression Models consisted of six different models and the full model, which was formulated by six combinations five resulting to, the under listed models below:

(a) $y \sim x_1 + x_2 + x_3 + x_5 + x_6$ …2
(b) $y \sim x_1 + x_2 + x_3 + x_4 + x_5$ …3
(c) $full\ model\ y \sim x_1 + x_2 + x_3 + x_4 + x_5 + x_6$ …4
(d) $y \sim x_2 + x_3 + x_4 + x_5 + x_6$ … 5
(e) $y \sim x_1 + x_2 + x_3 + x_4 + x_6$ … 6
(f) $y \sim x_1 + x_2 + x_4 + x_5 + x_6$ …7
(g) $y \sim x_1 + x_3 + x_4 + x_5 + x_6$ …8

Where x_1, x_2, x_3, x_4, x_5, x_6 represents S_iO_2, FeO, Fe_3O_4, CaO, Al_2O_3, Cu$_{\{matte\}}$, respectively, and y stands for Cu$_{\{slag\}}$.

3. Multiple Linear Regression MLR (p)

Multiple Linear Regression is a statistical technique that can be used to analyze the relationship between a single experimental variable and several explanatory variables. Moreover, regression method is one of the most widely used statistical techniques [31]. According to [32], regression analysis is one of the most commonly used statistical methodologies in many branches of science and engineering for discovering functional relationships between variables. The most typical example of regression analysis is Multiple Linear Regression modeling, which is used for predicting values of one or more response variables from any factor of interest, the independent variables. It has however received applications in almost every area of science, engineering and medicine. Moreover, the regression model is basically divided into two parts; the controlled part, which can be ascribed to all the observation considered as a group in a parametric framework and the stochastic part, which is the change between the observed and the expected values, which arises from the unknown sources [33]. More account of the theory and applications of linear regression model are discussed in [34], [35], [36], [20], [37], [38], [39], etc.

It has been on a literature that Multiple Linear Regression should not be confused or contradicted with Multivariate Linear Regression. Multivariate Linear Regression could be viewed as a linear relationship that exists between more than one experimental variables and sets of regressor variables [40]

The general form of Multiple Linear Regression model which aims at using the known variable to model and predict the unknown variable is shown below;

$$y_i = f(X_j, \beta) + \varepsilon_i \quad ; i = 1,2,\dots,p \qquad \dots 9$$

where p is the number of observation, $X_j = (x_{1i}, x_{2i}, \dots, x_{ki})$ is the vector of the predicted variable related to y_j

$\beta = (\beta_0, \beta_1, \dots, \beta_p)$ is the parameter vector and ε_i is the stochastic or random error associated with the ith observation reorganizing all the usual assumptions; See section (6.1), Linear Models in Statistics, Second edition by [30]. The parameters $\beta = (\beta_0, \beta_1, \dots, \beta_p)$ in the model, equation 1.1 can be estimated by Least Square Method of estimation since all the usual assumptions existed.

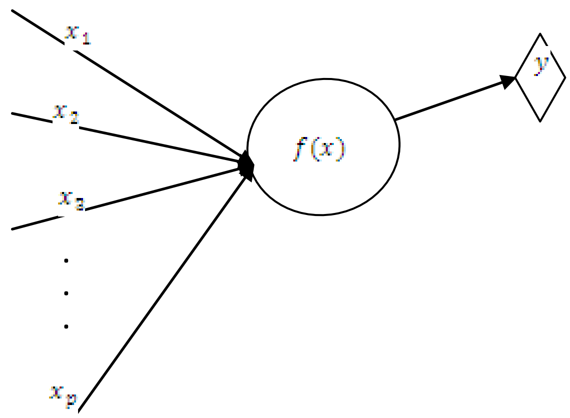
Equation …9 can equally be re-written as;

$$Y = X\beta + \varepsilon \qquad \dots 10$$

From equation …10, the estimate of the parameters of the model which were obtained by Least Square Method of parameter estimation was given by

$$\beta = (X'X)^{-1}X'y \qquad \dots 11$$

Equation …11 minimizes the sum of squares of the stochastic term. The predicted or expected model becomes $\hat{Y} = \hat{X}\beta$, so that the residual or error is given by $\hat{\varepsilon} = Y - \hat{Y}$.



3.1. Diagrammatic representative of Multiple Linear Regressions

Figure1: A sketch of the functional mapping of the explanatory variables to the explained variable.

Form the above figure, $f_{(x)}$ is a linear function which maps the sets of independent variables x_i to a response variable y. x_i are the sets of the independent variables and y is the explained variable. However, it is very similar to the functional mapping of Artificial Neural Networks, Multi-Layer Perceptron (MLP) case, only that the mapping function here is a linear function, which operates on the inputs (independent variables) to give the output (dependent variable).

3.2. R- Squared (R^2)

R-Squared denoted by R^2 is a statistical measure of how close the data are to the fitted regression line. It is also known as the coefficient of determination, or the coefficient of multiple determinations for Multiple Regressions. The definition of R-Squared is fairly straight forward; it is the percentage of the response variable variation that is explained by a linear model. That is;

$$R^2 = \frac{Explained\ Variation}{Total\ Variation}$$

$$\equiv \frac{MSS}{TSS} = 1 - \frac{RSS}{TSS} = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \quad ...12$$

$$\text{where } 0\% \leq R^2 \leq 100\%$$

0% indicates that the model explains none of the variability of the response data around its mean, while100% indicates that the model explains all the variability of the response data around its mean. In general, the higher the R-Squared the better the model fits your data.

However, in some fields of study, it is entirely expected that your R-Squared values will be low. For instance, any field of study that attempts to predict human behavior such as psychology, etc. and some other fields like technological processes, like smelting of copper slag, typically has R-Squared values lower than 5%. Humans and some other technological processes are very difficult to predict unlike physical processes, [41].

3.3. Predictive Error Sum of Squares $(PRESS)$

It is the sum of the squared differences between the experimental response *y* and the response *predicted* by the regression model, i.e. for an object that was not used for model estimation. It is defined as:

$$PRESS = \sum_{i=1}^{n}\left(y_i - \hat{y}_{i/i}\right)^2 \quad ...13$$

where the notation i/i indicates that the response is predicted by a model estimated when the i^{th} sample was left out from the training set. Therefore, an equivalent parameter to R^2 can be defined, using in place of RSS the quantity $PRESS$. This parameter is called cross-validated R^2 and the accepted symbols are $R^2{}_{cv}$ or Q^2:

$$R^2{}_{cv} \equiv Q^2 = 1 - \frac{PRESS}{TSS} = 1 - \frac{\sum_{i=1}^{n}\left(y_i - \hat{y}_{\frac{i}{i}}\right)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

$$Q^2 < 1 \quad ...14$$

For computation, $Q^2 = \frac{R^2}{S_y}$ where $S_y = std.dev.$

For bad predictive models, Q^2 can assume even negative values when $PRESS$ is greater than TSS, meaning that in prediction the model performs worse than the no-model estimate, i.e. the mean response of the training set. For more details on Q^2, consult [42], [43], [44].

3.4. Residual Sum of Squares (RSS)

It is the sum of the squared difference between the experimental response y and the response calculated by the regression model:

$$RSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \quad ... 15$$

If RSS is equal to zero the model is perfect, i.e. for all the *n* samples, the calculated responses coincide with the experimental responses. Obviously, RSS also depends on the measure unit used for the response. In practice, for the same model, if you multiply the experimental response for 10, RSS is 100 times greater, being a squared quantity.

3.5. Total Sum of Squares (TSS)

It is the total variance that a regression model can explain and is used as a reference quantity to calculate standardized quality parameters. Also denoted as SSY, it is the sum of the squared differences between the experimental responses and the average experimental response;

$$TSS \equiv SSY = \sum_{i=1}^{n}(y_i - \bar{y})^2 \quad ...16$$

TSS is assumed as a theoretical reference model where for each experimental response a constant value is calculated as the average experimental response. As for RSS, also TSS depends on the measure unit used for the response.

3.6. Error Standard Deviation (Std)

The standard deviation S_y is a statistical estimate of the error also accounting for the model degrees of freedom. This quantity is in the same unit of the response and is based on the fitting performance of the model, i.e. RSS. A more direct measure of the average error of the response estimates is the *Standard Deviation* and is denoted by S_y and is calculated by $s_y = \sqrt{\frac{RSS}{n-p}}$ where *n* is the number of samples, *p*' the number of model parameters (often given by *p* variables plus the intercept).

3.7. Variance Inflation Factor (VIF) and Tolerance Index (TI)

In statistics, the variance inflation factor (VIF) quantifies the severity of multicollinearity in an ordinary least squares regression analysis. It provides an index that measures how much the variance (the square of the estimate's standard deviation) of an estimated regression coefficient is increased because of collinearity. However, variance Inflation Factor (VIF) is a means to detect multicollinearities between the independent variables of a model. The In general, the VIF is calculated for all independent variables of a model. Variables showing the greater values are removed from the model. As a rule of thumb, the VIF of all variables should be less than 10 in order to avoid troubles with the stability of the coefficients, [1]. VIF equals 1 when the vector X_j is orthogonal to each column of the design matrix for the regression of X_j on the other covariates. By contrast, the VIF is greater than 1 when the vector X_j is not orthogonal to all columns of the design matrix for the regression of X_j on the other covariates. Some software calculates the tolerance which is just the reciprocal of the VIF. The choice of which to use is a matter of personal preference of the researcher. From basic idea is to try to express a particular variable X_j by a linear model based on all other independent variables. If the calculated model has a good fit, the tested variable xi is likely to be multicollinear to one or more of the other variables. According to [45], Variance Inflation Factor (VIF) and Tolerance Index are two measures that can guide a researcher in identifying MC and equally declares that The square root of the Variance Inflation Factor tells you how much larger the standard error is, compared with what it would be if that variable were uncorrelated with the other predictor variables in the model.

a mathematical point of view, the VIF measures the increase of the variance in comparison to an orthogonal basis. The VIF of the k^{th} variable is defined by the following formula**:**

$$VIF_j = \frac{1}{1-R_j^2} \qquad \ldots 17$$

R_j^2 is the R^2 statistic from the regression of X_j on the other covariates. Unfortunately, there is no well-defined critical value for what is needed to have a "large" VIF. Some authors, such as [46], suggest 10 as being large enough to indicate a problem. Moreover tolerance Index (TI) is evaluated by the formula**:**

$$\frac{1}{VIF_j} = 1 - R_j^2 \qquad \ldots 18$$

4. Results

The Fitted Linear Model of the Six Formulated Models

Full model	$y = 0.472 + 0\ .005x_1 + 0.004x_2 + 0.020x_3 - 0.001x_4 - 0.016x_5 + 0.001x_6$
Model four	$y = 0.374 + 0\ .005x_2 - 0.004x_3 + 0.023x_4 - 0.003x_5 + 0.001x_6$
Model seven	$y = 0.240 + 0\ .006x_1 + 0.019x_3 + 0.00x_4 - 0.13x_5 + 0.001x_6$
Model six	$y = 0.700 + 0\ .002x_1 - 0.004x_2 - 0.002x_4 - 0.019x_5 + 0.003x_6$
Model one	$y = 0.465 + 0\ .005x_1 - 0.004x_2 + 0.020x_3 - 0.016x_5 + 0.001x_6$
Model five	$y = 0.374 + 0\ .005x_1 - 0.004x_2 + 0.023x_3 - 0.003x_4 + 0.001x_6$

Table1.0: the table of the fitted linear models

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The Abridged Table of Results

R^2	$Std.Dev.\ (S_y^2)$	Q^2	$Sig.$	T.I	VIF	Model Equation	Model Selection
0.09	0.06245	0.360	0.317	0.9100	1.0989	$y \sim x_1 + x_2 + x_3 + x_5 + x_6$	Model Four
0.087	0.06254	0.348	0.335	0.9130	1.0953	$y \sim x_1 + x_2 + x_3 + x_4 + x_5$	Model Six
0.086	0.06297	0.343	0.441	0.9140	1.0941	$y \sim x_1 + x_2 + x_3 + x_4 + x_5 + x_6$	Full Model
0.073	0.06303	0.291	0.448	0.9270	1.0788	$y \sim x_2 + x_3 + x_4 + x_5 + x_6$	Model One
0.072	0.06303	0.287	0.448	0.9280	1.0776	$y \sim x_1 + x_2 + x_3 + x_4 + x_6$	Model Five
0.071	0.06304	0.283	0.449	0.9290	1.0764	$y \sim x_1 + x_2 + x_4 + x_5 + x_6$	Model Three
0.068	0.06322	0.270	0.497	0.9320	1.0730	$y \sim x_1 + x_3 + x_4 + x_5 + x_6$	Model Two

Table2.0: Table of Model comparison

Order of Model Performance Selection judging with its R-Squared R^2 and $Std.Dev.\ (S_y^2)$.

Model Equation	Model Selection	Order of Model Performances
$y \sim x_1 + x_2 + x_3 + x_5 + x_6$	Model Four	First
$y \sim x_1 + x_2 + x_3 + x_4 + x_5$	Model Six	Second
$y \sim x_1 + x_2 + x_3 + x_4 + x_5 + x_6$	Full Model	Third
$y \sim x_2 + x_3 + x_4 + x_5 + x_6$	Model One	Fourth
$y \sim x_1 + x_2 + x_3 + x_4 + x_6$	Model Five	Fifth
$y \sim x_1 + x_2 + x_4 + x_5 + x_6$	Model Three	Sixth
$y \sim x_1 + x_3 + x_4 + x_5 + x_6$	Model Two	Seventh

Table3.0: Table of Model selection

Assessment of the Model Performance for the Presence of Multicollinearity(MC)

Model Equation	Model Selection	Order of Model Performances
$y \sim x_1 + x_3 + x_4 + x_5 + x_6$	Model Two	First
$y \sim x_1 + x_2 + x_4 + x_5 + x_6$	Model Three	Second
$y \sim x_1 + x_2 + x_3 + x_4 + x_6$	Model Five	Third
$y \sim x_2 + x_3 + x_4 + x_5 + x_6$	Model One	Fourth
$y \sim x_1 + x_2 + x_3 + x_4 + x_5 + x_6$	Full Model	Fifth
$y \sim x_1 + x_2 + x_3 + x_4 + x_5$	Model Six	Sixth
$y \sim x_1 + x_2 + x_3 + x_5 + x_6$	Model Four	Seventh

Table4.0: Table of Multicollinearity assessment

5. CONCLUSION

From the Analysis carried out in this work, table 1.0 gave the result of the fitted linear models of the five formulated models from the full model (using combinatorial analysis) and itself. It can be observed clearly that in each of the fitted linear models shown in table 1.0, the contribution of each of the independent variables to the explained variable can be viewed. Some independent variables explained the response variable in a negative dimension while others contributed positively in explaining the observed variable. In model seven, a particular independent variable being the CaO (concentration of Calcium Oxide) had no contribution to the response variable and could be well removed from the model.

Moreover, the abridged table, represented in table 2.0 captured some of the important components of the Regression Analysis carried out in this work. It was observed that the values for R- Squared (R^2) was very low and could be explained from the basis that the experiment that gave birth to the data used in this work was a complex technological experiment (pyrometallurgical processes) which normally produces a very low R- Squared (R^2), in fact less than 5% in values, [41]. The values of the standard deviation was equally addressed in the same table and the values increases down the table, indicating that as we move down the table, the performance of the formulate models decreases and that can equally be seen in the values of their R- Squared (R^2). This particular result was explained in table 3.0, where the orders of the model performances were arranged based on their R-Square values and their standard deviation values.

Multicollinearity which was assessed by the Tolerance Index (TI) and Variance Information Factor(VIF), indicated that the multicollinearity encountered was still within the limit of acceptance according to [1]. The values of TI and VIF obtained were under control. Also the predictive power of each of the formulated models was checked by obtaining the values of their Q^2 which accounts that the higher the values of the Q^2, the better the predictive power of the model. From table 2.0, one could observe that as you move down the table, the predictive powers of the models decreases.

Finally, the researcher was kin analyzing the data in order to uncover some of all these parameters that could be used to judge Linear Regression Models which he has finally succeeded in reporting them in this work.

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