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Application of the Maximum Likelihood Approach to Estimation of Polynomial Regression Model

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ABSTRACT
The ordinary least squares (OLS) method had been extensively applied to estimation of different classes of regression model under specific assumptions. However, this estimation procedure OLS does not perform well with outliers and small sample sizes. As a result, this work considered the application of the maximum likelihood method for polynomial regression model using sample sizes as against the large sample assumption in OLS. The efficiency of the maximum likelihood (ML) estimation technique was put to test by comparing its model fit to that of the OLS using some real world data sets. The results of analysis of these data sets using both methods showed that the ML outperformed the OLS since it gave better estimates with lower mean square error (MSE) values in all the four data sets considered and higher coefficient of determination (R^2) values. Although, both methods resulted in overall good fit, but the ML is more efficient than the OLS because it resulted in lower MSE for small sample sizes.

KEYWORDS: Polynomial regression model (PRM)**,** Maximum Likelihood (ML), Ordinary Least Squares (OLS)**,** Mean square error (MSE), Unbiasedness, Robustness, Efficiency**.**

1.0 INTRODUCTION

Polynomial regression is a form of regression in which the relationship between the independent variable *x* and the dependent variable *y* is modeled as a k^{th} degree polynomial in *x*. Polynomial regression fits a nonlinear relationship between the value of *x* and the corresponding conditional mean of *y*, denoted as E(*y*|*x*), and has been used to describe nonlinear phenomena such as the growth rate of tissues, the distribution of carbon isotopes in lake sediments, and the progression of disease epidemics. Although, polynomial regression fits a nonlinear model to the data, as a statistical estimation problem, it is linear, in the sense that the regression function E(*y*|*x*) is linear in the unknown parameters that are estimated from the data. For this reason, polynomial regression is considered to be a special case of multiple linear regression. The design of an experiment for polynomial regression appeared in a 1974 paper of Gergonne. In the twentieth century, polynomial regression played an important role in the development of regression analysis, with a greater emphasis on issues of design and inference.

In polynomial regression, a dependent variable is regressed on the powers of the independent variables. It can also be used in those situations where the relationship between study and explanatory variables is curvilinear. Sometimes, a nonlinear relationship in a small range of explanatory variables can also be modeled by polynomials. When presented with a data set, it is often desirable to express the relationship between variables in the form of an equation. The most common method of representation is a k^{th} degree polynomial which takes the form

$$Y = a_k x^k + \ldots + a_1 x + a_0 + \varepsilon \qquad (1)$$

The above equation is often referred to as the general polynomial regression model with the error ε serving as a reminder that the polynomial will typically provide an estimate rather than an implicit value of the dataset for any given value of *x*. The predictors resulting from the polynomial expansion of the "baseline" predictors are known as interaction features. Such predictors or features are also used in classification settings. The maximum order of the polynomial is dictated by the number of data points used to generate it. For a set of *N* data points, the maximum order of the polynomial is $k=N-1$. However, it is generally best practice to use as low of an order as possible to accurately represent your dataset as higher order polynomials, while passing directly through each data point, can exhibit erratic behavior between these points due to a phenomenon known as polynomial wiggle.

Polynomial regression analysis has also been used across business fields for tasks as diverse as systematic risk estimation, production and statistical inference. Current practice in its teaching relies on the investigation of data sets for users with techniques that allow description and inference. There are many alternatives, however, for actual learner in the computation of regression coefficients and summary statistics. One of such was presented in Kmenta (1990**)** as a computational design that allows users to complete the calculations with only a pencil and paper, while it was suggested that learners might simply construct a scatter plot and a ruler to visually approximate the regression line. The use of statistical packages which are now easily accessible to users on mainframe and microcomputers was recommended also (Mundrake & Brown,1989). It is well known that if a regressor of a linear regression is measured with errors, the ordinary least squares (OLS), or naïve estimator of the corresponding slope parameter will be biased, the bias usually being such that it will attenuate the true value of the slope parameter (Cheng & Van Ness, 1999**)**.

The least squares method in the PRM, like other regression models, minimizes the variance of the unbiased estimators of the coefficients, under the conditions of the Gauss–Markov theorem. More recently, estimation of polynomial models has been complemented by different methods such as adjusted least squares, structural least squares and many more with certain inadequacies which are dealt with differently. It has been established that most of these methods present estimators with notable inadequacies. The most notable of these inadequacies are poor handling of outliers and small sample sizes. The latter leads to the violation of the OLS assumption on large samples and makes the validity of the procedure questionable. This motivates the application of the maximum likelihood (ML) estimator for modelling polynomial regression model in the presence of small samples.

2.0 MATERIALS AND METHODS

The application of ML technique for first order polynomial regression model of degree 2 and 3 polynomial regression models. The development of the ML technique entails the construction of the likelihood function on the response variable *Y* in (1) by assuming that it is Gaussian in nature. The log likelihood will be maximized with respect to each partial slope coefficient and the resulting system of equations will be solved simultaneously to obtain the ML estimate of each of the partial slope coefficients. The ML estimators will be fitted to some data sets which are characterized with small sample sizes. These data were would be subjected to exploratory analysis to affirm that they follow the appropriate polynomial (regression) order. The data sets are namely data of corrosion wheel set up, data of Nigerian PPP and GDP and data of output, total production cost of a commodity and electricity consumption data. The ML approach is used to fit the appropriate polynomial order to each of the data sets. The validity of the model fit (by ML approach) shall be tested by comparing its results with that of the OLS using their parameter estimates (partial slope coefficients), standard error estimates (of each partial slope), coefficients of determination and mean square error (MSE) values. In particular, the efficiency of the methods shall be tested using the coefficient of determination, test of significance (of parameters or variables) and MSE. The illustration and implementation shall be done by considering the problem of ten home sizes (sq ft) and their power consumption (KWh/month) reported in McClave & Deitrich (1991) as well as the data of total production cost and output of a commodity reported in Gujarati (2004) to mention a few. The analysis will be carried out using SAS (version 9.4).

3.0 APPLICATION OF THE MAXIMUM LIKELIHOOD APPROACH TO POLYNOMIAL REGRESSION MODEL

Polynomial regression is a special case of multiple regressions, with only one independent (predictor) variable *X*. One-variable polynomial regression model can be expressed as

$$Y_i = \beta_o + \beta_1 X_i + \beta_2 X_i^2 + \beta_3 X_i^3 + \dots + \beta_k X_i^k + \varepsilon \quad \text{for } i = 1, 2, \dots, n \qquad (2)$$

where Y_i is the response variable, X_i*'s are* the control variables , β_i*'s* are the partial slope parameters*,* ε_i is the stochastic disturbance (error) term which is Gaussian with expected value zero and common variance σ_i^2 and k is the degree of the polynomial. (2) is called the first order k^{th} degree polynomial which in fact is synonymous to (1).

Effectively, (2) is the same as having a multiple model with $X_1 = X$, $X_2 = X^2$, $X_3 = X^3$e.t.c

From (2), a first order polynomial regression model of degree (3) is

$$Y_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \beta_3 X_i^3 + \varepsilon_i \qquad (3)$$

Where the random error term is tagged as the random noise ε_i which is assumed to have a Gaussian distribution with mean zero and variance σ_i^2 i.e. N $(0, \sigma_i^2)$, so that four unknown parameters, $\beta_0, \beta_1, \beta_2$and β_3 are to be estimated using any given sample (data). Since X_i*'s* are thought of as fixed points and non-random, their randomness are dealt with using the noise variables ε_i , then for fixed X_i*'s,* the distribution of Y_i is also equal to $N(E(Y_i), \sigma^2)$ with p.d.f.

$$f(y) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(Y_i - \mu_i)^2 / 2\sigma^2} \qquad (4)$$

Since $\mu_i = E(Y_i) = \hat{Y}_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \beta_3 X_i^3$ (unbiasedness)

Then (4) can be written as

$$f(Y) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(Y-E(Y_i))^2/2\sigma^2} \quad (5)$$

so that the likelihood function of the random sample $Y_1, \ldots, Y_n$ can be written as

$$L = f(Y_1, \ldots, Y_n) = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^n e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}[Y_i - \hat{Y}(X_i)]^2} \quad (6)$$

So that (4) becomes

$$L = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^n e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 X_i - \beta_2 X_i^2 - \beta_3 X_i^3)^2} \quad (7)$$

Taking the natural logarithm of (5) yields the log likelihood

$$\ln L = \frac{n}{2}\ln 2\pi - \frac{n}{2}\ln\sigma^2 + \frac{1}{2\sigma^2}\sum_{i=1}^{n}(Y_i - \beta_0 - \beta_1 X_i - \beta_2 X_i^2 - \beta_3 X_i^3)^2 \quad (8)$$

The estimates of the parameters $\beta_0, \beta_1, \beta_2$ and β_3 are obtained by maximizing (8) w.r.t the parameters.The maximization of the log likelihood function w.r.t parameters $\beta_0, \beta_1, \beta_2$ *and* β_3 yields

$$\sum_{i=1}^{n} Y_i = n\beta_0 + \beta_1\sum_{i=1}^{n} X_i + \beta_2\sum_{i=1}^{n} X_i^2 + \beta_3\sum_{i=1}^{n} X_i^3 \quad (8a)$$

$$\sum_{i=1}^{n} X_i Y_i = \beta_0\sum_{i=1}^{n} X_i + \beta_1\sum_{i=1}^{n} X_i^2 + \beta_2\sum_{i=1}^{n} X_i^3 + \beta_3\sum_{i=1}^{n} X_i^4 \quad (8b)$$

$$\sum_{i=1}^{n} X_i^2 Y_i = \beta_0\sum_{i=1}^{n} X_i^2 + \beta_1\sum_{i=1}^{n} X_i^3 + \beta_2\sum_{i=1}^{n} X_i^4 + \beta_3 X_i^5 \quad (8c)$$

$$\sum_{i=1}^{n} X_i^3 Y_i = \beta_0\sum_{i=1}^{n} X_i^3 + \beta_1\sum_{i=1}^{n} X_i^4 + \beta_2\sum_{i=1}^{n} X_i^5 + \beta_3\sum_{i=1}^{n} X_i^6 \quad (8d)$$

(8a) to (8d) are solved simultaneously by transforming into the following matrix form

$$\begin{pmatrix} N & \sum_{i=1}^{n} X_i & \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 \\ \sum_{i=1}^{n} X_i & \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 \\ \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 & \sum_{i=1}^{n} X_i^5 \\ \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 & \sum_{i=1}^{n} X_i^5 & \sum_{i=1}^{n} X_i^6 \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{n} Y_i \\ \sum_{i=1}^{n} X_i Y_i \\ \sum_{i=1}^{n} X_i^2 Y_i \\ \sum_{i=1}^{n} X_i^3 Y_i \end{pmatrix} \quad (9)$$

Similarly, the parameters β_0, the intercept, β_1 the linear effect parameter, β_2 the quadratic effect parameter and β_3 the cubic effect parameter can then be obtained from (9) using Crammer's rule by seeking the determinants of a, a_0, a_1, a_2 and a_3 as follows

$$a = \begin{pmatrix} N & \sum_{i=1}^{n} X_i & \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 \\ \sum_{i=1}^{n} X_i & \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 \\ \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 & \sum_{i=1}^{n} X_i^5 \\ \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 & \sum_{i=1}^{n} X_i^5 & \sum_{i=1}^{n} X_i^6 \end{pmatrix}$$

$$a_0 = \begin{pmatrix} \sum_{i=1}^{n} Y_i & \sum_{i=1}^{n} X_i & \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 \\ \sum_{i=1}^{n} X_i Y_i & \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 \\ \sum_{i=1}^{n} X_i^2 Y_i & \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 & \sum_{i=1}^{n} X_i^5 \\ \sum_{i=1}^{n} X_i^3 Y_i & \sum_{i=1}^{n} X_i^4 & \sum_{i=1}^{n} X_i^5 & \sum_{i=1}^{n} X_i^6 \end{pmatrix}$$

$$a_1 = \begin{pmatrix} N & \sum_{i=1}^{n} Y_i & \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 \\ \sum_{i=1}^{n} X_i & \sum_{i=1}^{n} X_i Y_i & \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 \\ \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^2 Y_i & \sum_{i=1}^{n} X_i^4 & \sum_{i=1}^{n} X_i^5 \\ \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^3 Y_i & \sum_{i=1}^{n} X_i^5 & \sum_{i=1}^{n} X_i^6 \end{pmatrix}$$

$$a_2 = \begin{pmatrix} N & \sum_{i=1}^{n} X_i & \sum_{i=1}^{n} Y_i & \sum_{i=1}^{n} X_i^3 \\ \sum_{i=1}^{n} X_i & \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i Y_i & \sum_{i=1}^{n} X_i^4 \\ \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^2 Y_i & \sum_{i=1}^{n} X_i^5 \\ \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 & \sum_{i=1}^{n} X_i^3 Y_i & \sum_{i=1}^{n} X_i^6 \end{pmatrix}$$

$$a_3 = \begin{pmatrix} N & \sum_{i=1}^{n} X_i & \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 \\ \sum_{i=1}^{n} X_i & \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 \\ \sum_{i=1}^{n} X_i^2 & \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 & \sum_{i=1}^{n} X_i^5 \\ \sum_{i=1}^{n} X_i^3 & \sum_{i=1}^{n} X_i^4 & \sum_{i=1}^{n} X_i^5 & \sum_{i=1}^{6} X_i^6 \end{pmatrix}$$

yielding $\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2$ *and* $\hat{\beta}_3$ as

$\hat{\beta}_0 = \frac{\det(a_0)}{\det(a)}$, $\hat{\beta}_1 = \frac{\det(a_1)}{\det(a)}$, $\hat{\beta}_2 = \frac{\det(a_2)}{\det(a)}$ and $\hat{\beta}_3 = \frac{\det(a_3)}{\det(a)}$

which are estimates of β_0, β_1, β_2 and β_3. Similarly, for quadratic form, *estimates* $\hat{\beta}_0, \hat{\beta}_1$, and $\hat{\beta}_2$ can be obtained

4.0 ANALYSIS

Exploratory analysis involving the construction of scatter plot will be done. This allows visual approximation of each regression line and informs development of computational design that allows us to carry out its appropriate estimation (Kmenta, 1990). Each of the plots are presented as follows:

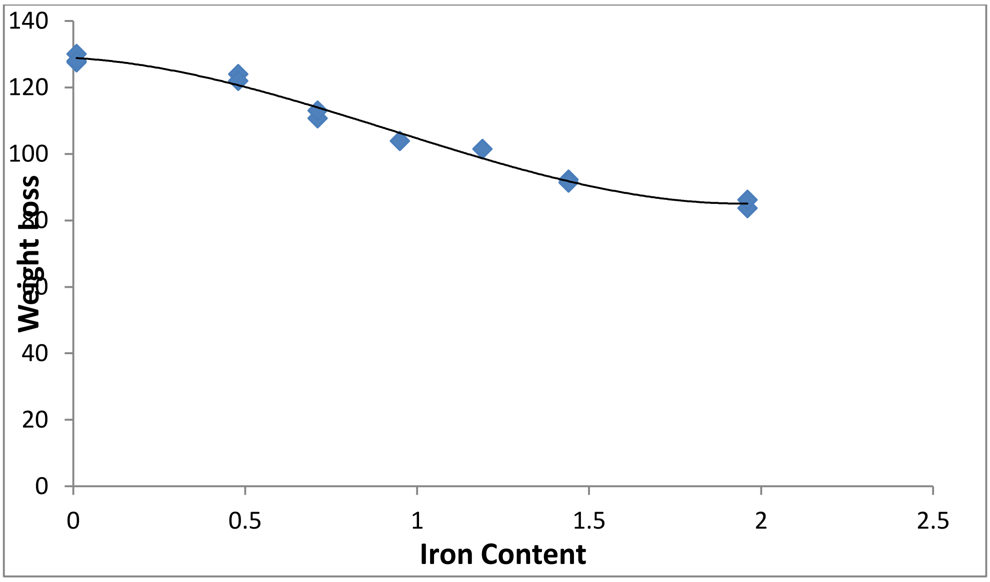

Fig 4.1- Graph of Iron corrosion data

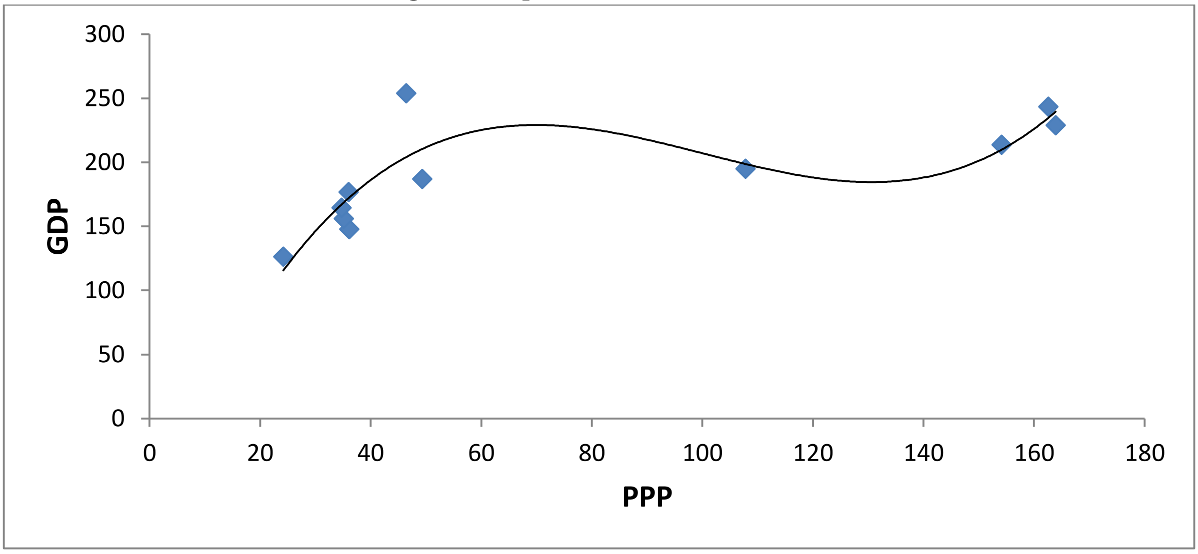

Fig 4.2 – Graph of Nigerian Gross Domestic Product (GDP) and Power Purchasing Parity (PPP) between 1989 and 1999

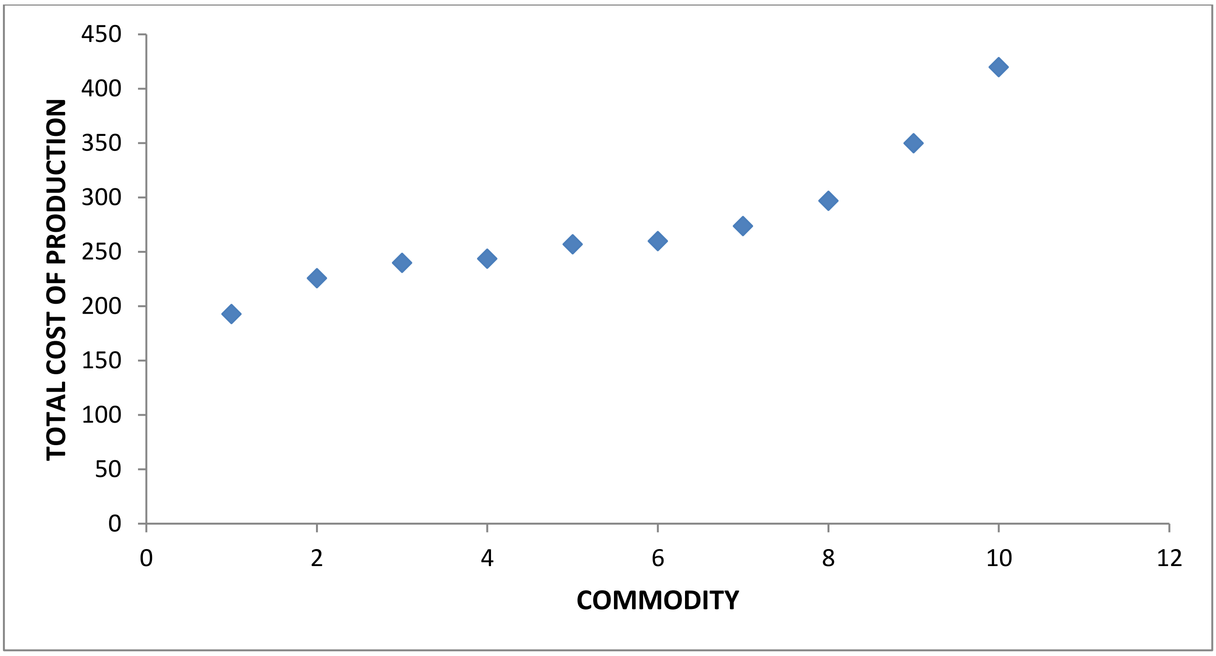

Fig 4.3-Graph of Total Production Cost and Output

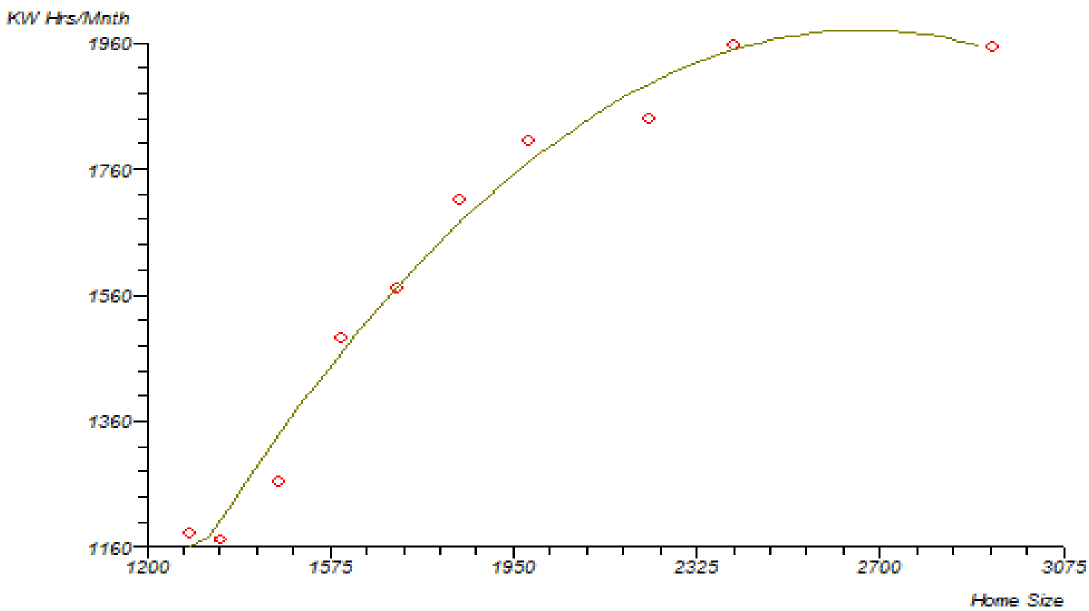

Fig 4.4-Graph of monthly Electricity consumption and home sizes

The exploratory analysis shows that each of these data sets either follows a quadratic or cubic order since their graphs show a sigmoid shape or parabola. This informs the use of cubic regression model for the iron corrosion data, PPP and GDP data, and output/total production cost data while the quadratic form was used for the data of home sizes and electricity consumption.

The ML technique was applied as an alternative to the traditional OLS since the OLS assumption of large samples is not met. The results of the analyses (by ML technique and that of the OLS) are presented for comparison. The parameter estimates, standard error (S.E.), t-ratios (for test of significance of each parameter), coefficient of determination R^2 value and the mean square error values for ML and OLS are presented in the table. These estimates give insights on the efficiency of the ML approach and overall goodness of fit. The table of comparison is presented below:

Tab 4.1-Table of Comparison

S/N	Datasets	No of samples	Estimates	MLE	OLS
1.	Data of Corrosion wheel set up	13	Parameters S.E P-value of /t/ R^2 value MSE value	β_0 β_1 β_2 β_3 128.889 -5.5244 -29.2076 10.5226 S.E(β_0) S.E(β_1) S.E(β_2) S.E(β_3) 1.325 6.972 9.288 3.174 0.0001 0.0485 0.0118 0.0090 0.9867 5.001	β_0 β_1 β_2 β_3 128.9489 -5.1956 -30.376 11.0086 S.E(β_0) S.E(β_1) S.E(β_2) S.E(β_3) 1.381 7.641 10.473 3.602 0.0001 0.0436 0.0176 0.01337 0.9858 5.429
2.	Data of PPP and GDP in Nigeria between 1989 and 1999	11	Parameters S.E P-value of /t/ R^2 value MSE value	β_0 β_1 β_2 β_3 3538.061 -61.6291 0.3478 -0.000625 S.E(β_0) S.E(β_1) S.E(β_2) S.E(β_3) 1117.598 18.5044 0.0998 0.00018 0.0158 0.0126 0.0102 0.0092 0.8245 831.2	β_0 β_1 β_2 β_3 3538.061 -61.6291 0.3478 -0.000625 S.E(β_0) S.E(β_1) S.E(β_2) S.E(β_3) 1117.59 18.504 0.0998 0.00018 0.0158 0.0126 0.0102 0.0092 0.8245 831.2
3.	Data of output and total production cost of a commodity	10	Parameters S.E P-value of /t/ R^2 value MSE value	β_0 β_1 β_2 β_3 141.767 63.4777 -12.9615 0.9396 S.E(β_0) S.E(β_1) S.E(β_2) S.E(β_3) 6.3753 4.778 0.986 0.059 0.0001 0.0001 0.0001 0.0001 0.9983 1.789	β_0 β_1 β_2 β_3 141.767 63.4777 -12.9615 0.9396 S.E(β_0) S.E(β_1) S.E(β_2) S.E(β_3) 6.3753 4.778 0.986 0.059 0.0001 0.0001 0.0001 0.0001 0.9983 1.8124
4	Data of home sizes and electricity consumption	10	Parameters S.E P-value of /t/ R^2 value MSE value	β_0 β_1 β_2 -1216.14389 2.39893 -0.00045 S.E(β_0) S.E(β_1) S.E(β_2) 43.235 0.8973 0.00002 0.0012 0.0001 0.0001 0.9875 1425.67	β_0 β_1 β_2 -1217.2341 2.41333 -0.0005 S.E(β_0) S.E(β_1) S.E(β_2) 44.576 0.9148 0.00005 0.0016 0.0001 0.0001 0.98125 2190.365

5.0 DISCUSSION OF RESULTS

The above table 4.1 presents the comparison between the MLE and OLS techniques the first order cubic regression and first order quadratic regression model using four data sets with small sample sizes. The comparison was carried out between the two methods using the parameter estimates, standard error estimates of each parameter, p-value of the student's t-ratios, coefficients of determination and the Mean Square error(MSE) values. The parameter estimates will give insight on bias of the estimates while the coefficient of determination and t-ratios will provide insight on the overall goodness of fit and detection of multicollinearity while the MSE values provides insight on the efficiency of the estimation technique.

The result of analysis of the first data set (of iron content and weight loss of some specimen tested in a corrosion wheel set up), show that the ML gave parameter estimates 128.889, -5.524, -29.208, 10.523 and the OLS resulted in 128.949, -5.196, -30.376, 11.009. Also, the ML resulted in standard error (SE) estimates 1.325, 6.972, 9.288, 3.174 while the OLS resulted in S.E estimates 1.381, 7.641, 10.473, 3.602. The ML has a slightly greater R^2 value of 0.987 (when compared to that of the OLS with 0.986) while a slightly lower MSE 5.005 of the ML indicated that the ML is more efficient that the OLS with MSE value of 5.429 with identical (exactly the same) decisions in their tests of significance of each of the parameters.

Furthermore, the analysis of the second data set (of Nigerian PPP and GDP between 1989 and 1999) showed that both methods gave identical parameter estimates 3538.06, -61.629, 0.3478, -0.000625, 3538.06, identical S.E estimates 1117.59, 18.504, 0.099, 0.00018 , identical R^2 value 0.8285 and identical MSE value of 831.2 with identically significant t-ratios.

The analysis of the third data set(on total production cost and output of a commodity) by showed identical parameter estimates, and different MSE values141.767 ,63.4777, -12.9615, 0.9396, identical S.E 6.3753, 4.778 ,0.986, 0.059, identical R^2 value of 0.9983 but lower MSE 1.789 (than 1.8124 for the OLS

The analysis of the last data set (on electricity consumption in kilo-watt-hours per month and home size of ten houses in square feet) showed that the MLE resulted in parameter estimates of -1216.1439, 2.3989, -0.000045, while the OLS resulted in parameter estimates-1217.2341, 2.41333 , -0.0005. The ML has S.E. estimates 43.235, 0.8973,0.00002 while the OLS resulted in S.E. 44.576, 0.9148, 0.00005, while the ML has a slightly higher R^2 value of 0.9875 (than the OLS with 0.9813) and a lower MSE 1425.67 (than 2190.365 for the OLS). Both resulted in identically significant t-ratios.

6.0 CONCLUSION

The result of the model fit of the four data sets using the ML resulted in reasonable parameter estimates (with lesser S.E relative to the parameter estimates), lower MSE, significant t-ratios and very high R^2 values. The latter two results indicated the absence of multicollinearity problem and an overall goodness of fit. The ML produced unbiased estimators for the OLS for three (out of the four) data sets considered since the ML estimates all coincided with that of the OLS in the three cases. The ML provided slightly different estimates from that of the OLS for the fourth data set which implies that there is a small bias in the fourth data set. However, the smaller the bias, the better the accuracy of the estimator and the estimator with the least bias is considered the best. The resulting parameter estimates by the ML showed little (in the fourth data) or no bias (in the other three data sets) which leads to the conclusion that the ML estimators are good estimators for the PRM.

In terms of goodness of fit, both estimators accounted for good fit because they both have high R^2 values and significant t-ratios but the ML gave a better fit since it resulted in higher R^2 values and lower MSE for all the data sets than the OLS technique. This latter quality ultimately leads to the conclusion that the ML is a more efficient technique for small samples than the OLS.

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