Assessment of Asymptotic and Logistics Growth Models on A Chemist Data

Onyinebifun Emmanuel Biu, Maureen Tobechukwu Nwakuya, and Gamage Tubona

Abstract — This research considers two growth models; asymptotic growth model and logistic growth model. Both models were compared to establish a better model for modelling and prediction based on a Chemist data on the percentage concentration of isomers versus time for each isomerization of α-Pinene at 189.5 °C. Results from the growth curve shows a non-linear relationship between the response (time of isomerization) and the independent variables (percentage of concentration) for all the four isomers considered. Based on the four isomers four different quadratic regressions of second-order were fitted. The problem of the initial parameters was addressed by second-order regression techniques since the models considered have three parameters to be estimated before the iterative approach was used. Estimation of parameters was done using modified version of the Levenberg-Marquardt Algorithm in Gretl statistical software. The results from both models were compared based on Aikaike Information Criteri (AIC), Bayesian Information Criteria (BIC), Mean Squared Error (MSE) and R-square. The Asymptotic Growth Model was identified to be a more adequate model for modelling and predicting growth patterns for three isomers (Dipentene, Pyronene and Dimer) while logistic growth model was seen to be a better model for predicting growth patterns of one isomer (Allo-Ocimene). This study will go a long way in directing Chemists and researchers in that field in choosing the appropriate model for their research.

Keywords — Asymptotic Growth Model; Levenberg-Marquardt Algorithm; Logistic Growth Model and Non-linear Model.

1. INTRODUCTION

Regression models explain the dependence relationship between a response random variable and a set of explanatory variables. Regression analysis helps investment and financial managers to value assets and understand the relationships between variables, such as commodity price and the stocks of businesses dealing in those commodities. Given n-dimensional independent random variables \(x_1, x_2, x_3, \ldots, x_n\) the regression models specifies the conditional distribution of \(y|x_1, x_2, x_3, \ldots, x_n\). Specifically, a regression method principally is concerned with the mean of this distribution: \(E(Y|x_1, x_2, x_3, \ldots, x_n)\) which is the conditional expectation of the response variable given the explanatory variables and it is known as the regression function. The mean regression can be linear or non-linear regression. Nonlinear regression models are indispensable tools for statistical analysis when the assumption of linearity fails. There are situations where theoretically nonlinear regression is suitable such as, in animal growth from birth to adulthood, this is clearly nonlinear since such growth could be rapid soon after birth and leveling off at adulthood [1]. In the biological sciences, the growth curves have numerous significant applications, the growth regression models have been found to give a good description of different growth patterns exhibited by variables.

Nonlinear regression models are also used in social sciences, physical, engineering, biological, management sciences, business and economics. Reference [2] estimated the parameters of two non-linear regression models using iterative steps to fit model with data sets. A lot of nonlinear regression models have been derived by mathematicians and statisticians. Most of these models have been applied to different real data sets according to different research problems in the different fields of study. On the other hand, there are a huge number of circumstances in the real life setting where the application of nonlinearly regression models becomes difficult because of intractability of the statistical model. This could be due to the fact that a great number of nonlinear regression models have been proposed by statistician thus, determining the appropriate nonlinear model for a particular data set becomes a difficult task. Also, the problem of lack of fit of a statistical model could be traced to fitting a data set to an inappropriate model.

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Method of estimating the parameter of the nonlinear regression model has been identified as a critical issue in the utilization of the nonlinear regression models. Reference [3] described some computational methods based on numerical analysis to estimate the parameters of nonlinear regression model. In this study, two nonlinear regression models are studied: the logistic growth regression model and the asymptotic growth regression. The study applied the estimation of the parameters of a nonlinear regression model using an assumed initial values and a modified version of the Levenberg-Marquardt Algorithm in Gretl statistical software to model a chemist data using two growth models.

II. GROWTH MODELS

A. Logistic Growth Model

The logistic growth model is used in modelling nonlinear relationships, like population growth and likes. Population growth is basically exponential in nature. Growth at an early stage will run very slowly, then it will rise sharply and when it approaches the maximum capacity, its growth will slow down again until it reaches zero growth. This growth model is an improvement from the exponential growth model which assumes the population will grow indefinitely, as hinted by [4]-[7].

In real life situations, it is out of question to have event grow exponentially forever. Thus, the exponential model approaches some limiting value if the growth drops significantly. For such growth, the logistic growth model becomes more appropriate. This scenario makes it obvious that the logistic growth model is first exponential and then records the down-step in growth rate as the response variable approaches the model’s upper bound. Generally, the appropriateness of a logistic growth model in the estimation of maximum rate of increase or optimum x level for maximizing the y value is a significant component of its function [8] and [9]. Reference [10] applied logistic regression to evaluate the association of driver characteristics and accident severity in Italy. The results indicated that males are more likely to be engaged in fatal accidents and that car drivers are less likely to be fatally injured than killed than motorcycle drivers.

The logistic model for one predictor variable is;

\[ y_i = \frac{\beta_0}{1 + \beta_1 \exp(\beta_2 x_i)} + \mu_i \]  (1)

In (1) \( \beta_0, \beta_1, \) and \( \beta_2 \) are the model parameters. The logistic model is hinged on the belief that growth rate is proportional to the population of interest and the remaining resources available to the existing population. The logistic growth model be expressed as

\[ y(t) = \frac{\beta}{1 + \exp(-\alpha(t-t_{inf}))} = \frac{\beta}{1 + \exp(-\alpha(t-t_{inf}))} \]  (2)

where: \( t_{inf} = \frac{1}{\alpha} \left( \frac{1}{\beta_0} - 1 \right) \)  (3)

Some of the applications of logistic growth model include; Reference [11], he examined the applicability of the logistic growth model in the study of the COVID-19 pandemic and other infectious diseases in multiple regions in China and other selected countries. The study showed that growth rate of out breaks was different for different regions and countries. The model showed a good fit and identified the existence of heteroscedasticity and positive serial correlation within residuals in some province and countries. Also [12] in a study to determine factors affecting diabetes in the red sea state used the logistic regression models and he observed that there was a relationship between diabetes infections and some predictor variables after analyzing data with simple binary logistic regression and multiple logistic regression.

B. Asymptotic Growth Model

The Asymptotic growth model is a nonlinear regression model that poses a deterministic component that is said to belong to the family of convex/concave curves that do not have any maxima or minima or a point of inflexion. It does not have the property of being transformed into a model form that is linear in parameters; hence it is inherently considered a nonlinear model. The estimation of the model parameters cannot be done using the widely favored least squares method. The asymptotic growth model is used to describe growth that is limited. When using asymptotic model, as the independent variable approaches infinity, the response variable tends to the horizontal asymptote. Different parameterization of the asymptotic growth model exists, in this study the following parameterization is considered

\[ y = \beta_0 + \beta_1 e^{\beta_2 x} \]  (4)
III. METHODS

This section describes the asymptotic growth model, the logistic growth models and estimation procedures applied in the study. The study made use of a chemist data that comprises of percentage concentration and time of isomerization of α-Pinene at 189.50 °C for four different isomers namely; Dipentene, Allo-Ocimene, Pyronene and Dimer. Because of the four different isomers, four quadratic regressions were considered. The quadratic model of second-order was used applied to obtain the initial value of the parameters for iterative approach and also the quadratic trend was plotted. Estimation of parameters was done using modified version of the Levenberg-Marquardt Algorithm in Gretl statistical software. The results from both models were compared based on Aikaike Information Criteri (AIC), Bayesian Information Criteria (BIC), Mean Squared Error (MSE) and R-square.

A. Statistical Properties of Logistic model

B A simple logistic growth model with the following model specification is considered:

\[ y(t) = \frac{\beta_0}{1 + e^{(\beta_1 + \beta_2)X}} \]  \hspace{1cm} (5)

Where: \( \beta_0 \) = growth rate, \( \beta_1 \) = upper asymptotes where the independent variable tends to infinity and \( \beta_2 \) is the growth range

The growth rate is obtained by taking the derivative of (5) with respect to \( x \)

\[ \frac{dy(t)}{dx} = \frac{-\beta_0 \beta_2 e^{(\beta_1 + \beta_2)X}}{(1 + e^{(\beta_1 + \beta_2)X})^2} \]  \hspace{1cm} (6)

The linear form of (5) is derived as follows;

\[ y(t)^+ = \frac{1 + e^{(\beta_1 + \beta_2)X}}{\beta_0} \Rightarrow \beta_0 y(t) = 1 + e^{(\beta_1 + \beta_2)X} \]  \hspace{1cm} (7)

\[ \ln \left( \frac{\beta_0}{y(t)} - 1 \right) = \beta_1 + \beta_2 \]  \hspace{1cm} (8)

B. Asymptotes of Logistic Growth Regression

Firstly, the parameters \( \beta_1 \) and \( \beta_2 \) are taken to be zero

\[ \beta_1 = 0 \Rightarrow y = \frac{\beta_0}{1 + \beta_0 \beta_2 X} \]  \hspace{1cm} (9)

\[ \beta_2 = 0 \Rightarrow y = \frac{\beta_0}{1 + \beta_0 \beta_1 X} \]  \hspace{1cm} (10)

C. Point of Inflection of Logistic Growth Regression Model

In Practice, growth curve modeling employing functions with an oblique asymptote and one or more inflection points is useful, [13].

From equation (7) we, have that; \( y(t) = \beta_0 (1 + e^{(\beta_1 + \beta_2)X})^{-1} \)

Hence, \( y'(t) = \frac{-\beta_0 \beta_2 e^{(\beta_1 + \beta_2)X}}{(1 + e^{(\beta_1 + \beta_2)X})^2} \)  \hspace{1cm} (11)

And, \( y''(t) = \frac{-\beta_0 \beta_2 e^{(\beta_1 + \beta_2)X}}{(1 + e^{(\beta_1 + \beta_2)X})^2} \)  \hspace{1cm} (12)

By taking the log of both sides we have; \( x = \frac{-\beta_1}{\beta_2} \)

D. Maximum Growth Rate

To obtain the maximum growth rate the value of \( x \) at the inflection point is obtained thus;

\[ \frac{dy(t)}{dx} = \frac{-\beta_0 \beta_2 e^{(\beta_1 + \beta_2)X}}{(1 + e^{(\beta_1 + \beta_2)X})^2} \]  \hspace{1cm} (13)

E. Relative Growth Rate

Relative Growth rate is a standardized measure of growth with the benefit of avoiding, as far as possible, the inherent differences in scale between contrasting organisms so that their performances can be compared on an equitable basis [14]. In this section, the relative growth is derived as a function of the independent variable
The parameters of the logistic regression model could be estimated using the method of maximum likelihood as follows. Let the likelihood function be;

\[ l = \prod_{i=1}^{n} f(y) = \prod_{i=1}^{n} \left( \frac{\alpha_i}{\alpha_i + (1-\alpha_i)^{1+y_i}} \right)^{y_i} \]

(15)

By taking the log of the likelihood function we have

\[
l = \log \left( \prod_{i=1}^{n} \left( \frac{\alpha_i}{\alpha_i + (1-\alpha_i)^{1+y_i}} \right)^{y_i} \right) = \sum_{i=1}^{n} y_i \log \left( \frac{\alpha_i}{\alpha_i + (1-\alpha_i)^{1+y_i}} \right) + \sum_{i=1}^{n} \log \left( \frac{\alpha_i}{\alpha_i + (1-\alpha_i)^{1+y_i}} \right) = y_i \log \left( \frac{\alpha_i}{\alpha_i + (1-\alpha_i)^{1+y_i}} \right) + \sum_{i=1}^{n} \log \left( \frac{\alpha_i}{\alpha_i + (1-\alpha_i)^{1+y_i}} \right) \]

(16)

Since, \( \alpha_i = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x_1 + \beta_2 x_2)}} \). It follows that \( 1 - \alpha_i = 1 + e^{(\beta_0 + \beta_1 x_1 + \beta_2 x_2)} \)

Hence;

\[
\log \left( \frac{\alpha_i}{\alpha_i + (1-\alpha_i)^{1+y_i}} \right) = y_i \log \left( 1 + e^{(\beta_0 + \beta_1 x_1 + \beta_2 x_2)} \right) + \sum_{i=1}^{n} \log \left( 1 + e^{(\beta_0 + \beta_1 x_1 + \beta_2 x_2)} \right)
\]

(17)

The MLE of the parameters are the values of \( \beta_0, \beta_1, \beta_2 \) that maximizes the likelihood of the function. No closed-form solution exists for the \( \beta_i \)'s in (4), consequently the estimates of the model parameters are obtained by computer numerical search techniques.

G. Estimation of Parameters using Assumed Value

In this method, we first assign an initial value to one of the parameters \( \beta_2 \) of the model. Secondly, a linear model is developed from the nonlinear regression equation. The transformed model is used to estimate the other parameters of the model where \( \beta_2 \) is assumed to lie \(-1, 0 \leq \beta_2 \leq 1\).

H. Asymptotic Growth Model

The asymptotic growth model for this study used the following parameterization;

\[ y = \beta_0 + \beta_1 x + \beta_2 x^2, \]

as shown in (4).

I. Statistical Properties of the Asymptotic Growth Model

To obtain the growth rate, (4) is differentiated with respect to \( x \). The linear form of (4) is obtained as follows:

\[ \ln y = \ln \beta_0 + \ln \beta_1 + \beta_2 x, \]

(18)

J. Asymptotes of Asymptotic Growth Model

When \( \beta_1 = 0, y = \beta_0 \) and when \( \beta_2 = 0, y = \beta_0 + \beta_1 \)

K. Asymptotic Growth Model

The research used the modified version of the Levenberg-Marquardt Method. The procedure is as follows;

1. Obtain partial derivation of the model with respect to the four parameters \( \beta_0, \beta_1, \beta_2 \)
2. Develop a program in the Gretl software using equation (4) and (5) and input the initial values by fitting second order polynomial (Quadratic Model), use Micro-Excel software for scatter plot and trend analysis.
3. Then substitute the coefficient \( \beta_0^{(0)}, \beta_1^{(0)}, \beta_2^{(0)} \) as initial guess values for iteration process.
4. Input the data and initiate guess values on the developed program. Then, run the iteration to obtain the results.

IV. DATA COLLECTION AND ANALYSIS

To assess and compare the behaviours of asymptotic and logistic growth models, data on percentage concentration and time for the Isomerization of \( \alpha \)-Pinene at 189.5°C in Table 1 was used, while applying the non-linear least squares estimation using a modified version of the Levenberg – Marquardt algorithm. The comparison was done based on the following model criteria; Aikake Information Criteria (AIC), Bayesian Information Criteria (BIC), Mean Squares Error (MSE) and Rsquared.
TABLE I: DATA ON PERCENTAGE CONCENTRATION AND TIME FOR THE ISOMERIZATION OF \( \alpha \)-PINENE AT 189.5 °C

| Time (Min) | Dipentene | Allo-Ocimene | Pyronene | Dimer |
|------------|-----------|--------------|----------|-------|
| 1230       | 7.3       | 2.3          | 0.4      | 1.75  |
| 3060       | 15.6      | 4.5          | 0.7      | 2.8   |
| 4920       | 23.1      | 5.2          | 1.1      | 5.8   |
| 7800       | 32.9      | 6.0          | 1.5      | 9.3   |
| 10680      | 42.7      | 6.0          | 1.9      | 12.0  |
| 15030      | 49.1      | 5.9          | 2.2      | 17.0  |
| 22620      | 57.4      | 5.1          | 2.6      | 21.0  |
| 36420      | 63.1      | 3.8          | 2.9      | 25.7  |

Taking partial derivation of asymptotic growth model in (4) with respect to \( \beta_0, \beta_1, \beta_2 \) we have,

\[
\frac{\partial y}{\partial \beta_0} = 1\quad (19)\\
\frac{\partial y}{\partial \beta_1} = e^{\beta_1 x}\quad (20)\\
\frac{\partial y}{\partial \beta_2} = \beta_2 x e^{\beta_2 x}
\]

A simple logistic growth model with the following mode specification is considered:

\[
y = \frac{\beta_0}{1 + e^{(\beta_0 + \beta_2 x)}} = \beta_0 \left(1 + e^{(\beta_0 + \beta_2 x)}\right)^{-1}\quad (21)
\]

Taking logarithm of both sides

\[
\ln(y) = \ln(\beta_0) - \ln\left(1 + e^{(\beta_0 + \beta_2 x)}\right)
\]

Let \( \alpha_0 = \ln(\beta_0), \alpha_1 = \beta_1 \) and \( \alpha_2 = \beta_2 \), we have

\[
Y = \alpha_0 - \ln\left(1 + e^{(\alpha_1 + \alpha_2 x)}\right)\quad (22)
\]

By taking partial derivation with respect to \( \alpha_0, \alpha_1, \alpha_2 \) we have,

\[
\frac{\partial y}{\partial \alpha_0} = 1\quad (23)\\
\frac{\partial y}{\partial \alpha_1} = -\left(1 + e^{(\alpha_1 + \alpha_2 x)}\right)^{-1} \ln\left(1 + e^{(\alpha_1 + \alpha_2 x)}\right)\\
\frac{\partial y}{\partial \alpha_2} = -x \left(1 + e^{(\alpha_1 + \alpha_2 x)}\right)^{-1} \ln\left(1 + e^{(\alpha_1 + \alpha_2 x)}\right)\quad (24)
\]

We now apply the modified version of the Levenberg-Marquardt Method to estimate the models

V. RESULTS AND DISCUSSIONS

A. Fitted second order polynomial (Quadratic Model) of each Isomerization of \( \alpha \)-Pinene at 189.50°C

![Fig. 1. Quadratic Trend Plot Y₁ Dipentene.](image)

The quadratic trend plots in Fig. 1 shows a curve not a straight line which reveals a non-linear relationship between percentage concentrations versus time on Isomerization. It is also noticed from the graph that the quadratic model fitted the data very well because all the observed data fits into the curve and it has R-squared of 98.95%, which confirms a very good fit. This plot also describes the shape of the asymptotic
growth curve. Hence we can say that percentage concentration versus time on Isomerization of α-Pinene at 189.5 °C to Dipentene exhibited asymptotic growth.

The quadratic trend plot in Fig. 2 shows a curve not a straight line which reveals a non-linear relationship between percentage concentrations versus time on Isomerization. It is also noticed from the graph that the quadratic model didn’t fit the data very well because all the observed data did not fit into the curve and it has R-squared of 64.44%, which confirms a slightly good fit. This plot has an S-shape that describes the shape of the logistic growth curve. Hence we can say that percentage concentration versus time on Isomerization of α-Pinene at 189.5 °C to Allo-Ocimene exhibited a logistic growth.

The quadratic trend plot in Fig. 3 also shows a curve which reveals a non-linear relationship between percentage concentrations versus time on Isomerization. It is also noticed from the graph that the quadratic model fitted the data very well because all the observed data fits into the curve and it has R-squared of 99.09%, which confirms a very good fit. This plot also describes the shape of the asymptotic growth curve. Hence we can say that percentage concentration versus time on Isomerization of α-Pinene at 189.5 °C to Pyronene exhibited asymptotic growth.

The quadratic trend plot in Fig. 4 shows a curve which reveals a non-linear relationship between percentage concentrations versus time on Isomerization. It is also noticed from the graph that the quadratic model fitted the data very well because all the observed data fits into the curve and it has R-squared of 99.09%, which confirms a very good fit. This plot also describes the shape of the asymptotic growth curve. Hence we can say that percentage concentration versus time on Isomerization of α-Pinene at 189.5 °C to Dimer exhibited asymptotic growth.
The quadratic trend plot in Fig. 4 shows a curve-linear relationship between percentage concentrations versus time on Isomerization. It is also noticed from the graph that the quadratic model fitted the data very well because all the observed data fits into the curve and it has R-squared of 99.65%, which confirms a very good fit. This plot also describes the shape of the asymptotic growth curve. Hence we can say that percentage concentration versus time on Isomerization of α-Pinene at 189.5 °C to Dimer exhibited asymptotic growth.

| Model Statistics | Asymptotic Growth Model Estimated coefficient (P-values) | Logistic Growth Model Estimated coefficient (P-values) | Best Fit |
|------------------|----------------------------------------------------------|--------------------------------------------------------|----------|
| Alpha(β₁)        | 4.0798 (0.0000*** )                                     | 4.2068 (0.0000*** )                                    | Asymptotic Growth Model |
| Beta(β₂) for X   | -2.6143 (0.0000*** )                                    | 2.1918 (0.0000*** )                                    |          |
| Beta(β₃) for X²  | -2.0138x10⁻³ (0.000*)                                   | -0.0034806 (0.0000*** )                                |          |
| MSE              | 0.0201                                                  | 0.0678                                                |          |
| BIC              | -18.9631                                                | -9.2014                                               |          |
| AIC              | -19.2014                                                | -9.4398                                               |          |
| R²               | 99.48%                                                  | 98.23%                                                |          |
| Iteration        | 27                                                      | 20                                                    |          |

Footnote: Sig at *0.10, **0.05, ***0.01

Table II indicates that Asymptotic Growth Model presented the lowest BIC, AIC and MSE, with the highest values of R-squared. Hence, Asymptotic Growth Model fitted the data for percentage concentrations versus time on Dipentene better than the logistic regression.

| Model Statistics | Asymptotic Growth Model Estimated coefficient (P-values) | Logistic Growth Model Estimated coefficient (P-values) | Best Fit |
|------------------|----------------------------------------------------------|--------------------------------------------------------|----------|
| Alpha(β₁)        | 5.3657 (0.0000*** )                                     | 1.6674 (0.0000*** )                                    | Logistic Growth Model |
| Beta(β₂) for X   | -8.0140 (0.2987)                                         | 1.6489 (0.1495)                                        |          |
| Beta(β₃) for X²  | -0.0077634 (0.2885)                                      | -1.1232x10⁻³ (0.1806)                                  |          |
| MSE              | 3.6660                                                   | 0.1552                                                |          |
| BIC              | 22.6987                                                 | -2.6004                                               |          |
| AIC              | 22.4603                                                 | -2.8387                                               |          |
| R²               | 68.77%                                                   | 79.30%                                                |          |
| Iteration        | 72                                                       | 21                                                    |          |

Footnote: Sig at *0.10, **0.05, ***0.01

Table III indicates that Logistic Growth Model presented the lowest BIC, AIC and SSE, with the highest values of R-squared. Therefore logistic Growth Model fitted the data for percentage concentrations versus time on Allo-Ocimene better than the asymptotic growth regression.

| Model Statistics | Asymptotic Growth Model Estimated coefficient (P-values) | Logistic Growth Model Estimated coefficient (P-values) | Best Fit |
|------------------|----------------------------------------------------------|--------------------------------------------------------|----------|
| Alpha(β₁)        | 3.0269 (0.0000*** )                                     | 0.9557 (0.0000*** )                                    | Asymptotic Growth Model |
| Beta(β₂) for X   | -2.9578 (0.0000*** )                                    | 1.9853 (0.0000*** )                                    |          |
| Beta(β₃) for X²  | -8.6185x10⁻⁵ (0.0000*)                                   | -0.0030374 (0.0000*** )                                |          |
| MSE              | 0.0074                                                   | 0.0454                                                |          |
| BIC              | -26.9118                                                 | -12.4271                                              |          |
| AIC              | -27.1501                                                 | -12.6654                                              |          |
| R²               | 99.86%                                                   | 98.63%                                                |          |
| Iteration        | 20                                                       | 20                                                    |          |

Footnote: Sig at *0.10, **0.05, ***0.01

Table IV indicates that Logistic Growth Model presented the lowest BIC, AIC and SSE, with the highest values of R-squared. Therefore Asymptotic Growth Model fitted the data for percentage concentrations versus time on Pyronene better than the Logistic growth regression.

Table V indicates that Logistic Growth Model presented the lowest BIC, AIC and SSE, with the highest values of R-squared. Therefore Asymptotic Growth Model fitted the data for a percentage concentration versus time on Dimer isomer is better than the logistics growth regression.
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interpretation and relating it to real life issues. Her quest for collaboration and knowledge propelled her to join many societies and academic bodies which includes; International Biometric Society, Royal Statistical Association, Nigerian Statistical Association, Nigerian Mathematical Society, Organization of Women in Sciences for the Developing Countries and International Association of Applied Econometrics.

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