Parameter estimation of Monod model by the Least-Squares method for microalgae *Botryococcus Braunii* sp

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Abstract. This research aims to estimate the parameters of Monod model of microalgae *Botryococcus Braunii* sp growth by the Least-Squares method. Monod equation is a non-linear equation which can be transformed into a linear equation form and it is solved by implementing the Least-Squares linear regression method. Meanwhile, Gauss-Newton method is an alternative method to solve the non-linear Least-Squares problem with the aim to obtain the parameters value of Monod model by minimizing the sum of square error (SSE). As the result, the parameters of the Monod model for microalgae *Botryococcus Braunii* sp can be estimated by the Least-Squares method. However, the estimated parameters value obtained by the non-linear Least-Squares method are more accurate compared to the linear Least-Squares method since the SSE of the non-linear Least-Squares method is less than the linear Least-Squares method.

1. Introduction

In 2050, the world population is estimated around nine billion people which are 1.5 times of the current population. Hence, the demand for commodities will rise explosively [1]. Sustainable production methods are necessary to develop and to exploit in order to supply the demand for commodities. Cultivation of microalgae plays an important role in the bio-based economy. Moreover, microalgae have high potential as a source of environmentally sustainable transport fuel because of their high oil content and rapid biomass production [2]. Besides that, microalgae can be cultivated to produce a variety of products such as plastics, chemical feedstock, lubricants, fertilizers and cosmetics [3]. Since the cultivation of microalgae has a huge contribution for sustainable production of food and energy, thus it is vital to study about the microalgae growth system. A mathematical modelling is required to describe the growth in microalgae cultivation. Michaelis-Menten or Monod model which was proposed by Jacques Monod in 1942 is one of the model used to estimate the specific growth of microalgae. Parameters consist in the Monod model widely influence in the microalgae cultivation system. Therefore, this research aims to estimate the kinetic parameters of Monod model by implementing the Least-Squares method.

2. Mathematical Modeling and Kinetic Expression

There are many mathematical models used to describe the microalgae growth system. The microalgae growth model was developed depends on the different input factors. The primary factors that have been experimentally and theoretically shown to affect the productivity of microalgae are light intensity, photosynthetic rate, respiration rate, temperature, nutrient availability and lipid production [4]. In this
research, we only focused on two correlated variables which are the light intensity and the saturation constant. These data are taken from [5]. The light intensity is selected as the primary factor which influences microalgae Botryococcus Braunii sp growth rate. Moreover, kinetic studies will be carried out to describe the microalgae growth production. Monod model is one of the kinetic growth models which can be expressed as [6]

$$\mu = \mu_{\text{max}} \frac{I}{I + K_I},$$

(1)

where $\mu$ represents the specific growth rate, $\mu_{\text{max}}$ is the maximum specific growth rate, $I$ is the light intensity and $K_I$ is the saturation constant for light intensity.

3. Least-Squares Method

The Least-Squares method is widely used to estimate the numerical values of the parameters by fitting a function to a set of measured data. The Least-Squares method aims to find the optimum when the sum of square error (SSE) is minimized. The $SSE$ is defined as

$$SSE = \sum_i r_i^2,$$

(2)

where

$$r_i = y_i - f(x_i, \beta_i).$$

(3)

When the $SSE$ approximates to zero, this means that the estimated parameter is close or equivalent to actual value. In Equation (3), if $f(x_i, \beta_i)$ is a linear function, then it is called as linear Least-Squares. However, when $f(x_i, \beta_i)$ is a non-linear function then it is a non-linear Least-Squares. For linear models, the Least-Squares minimization is solved analytically by applying simple calculus. Meanwhile, the minimization process of the non-linear model is done by an iterative numerical algorithm.

3.1. Least-Squares linear regression method

The linear Least-Squares regression equation can be described as [7]

$$\hat{Y} = a + bx,$$

(4)

where $\hat{Y}$ is a dependent variable, $x$ represents an independent variable, $a$ is an unknown regression parameter coefficient representing the intercept and $b$ is another unknown regression parameter coefficient representing slope.

The Least-Squares method is implemented to predict the parameters of the Monod model based on the experimental data and applying a certain objective function. The objective function is the $SSE$ of the observations $y_i$ from the true regression line which is defined as

$$SSE = \sum_i (y_i - \hat{Y})^2.$$  

(5)

Through solve the partial derivative $\frac{\partial SSE}{\partial a} = 0$ and $\frac{\partial SSE}{\partial b} = 0$, coefficients of $a$ and $b$ can be represented as [8,9]

$$a = \bar{y} - b\bar{x},$$

(6)

$$b = \frac{S_{xy}}{S_{xx}},$$

(7)
\[
\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n}, \quad \bar{y} = \frac{\sum_{i=1}^{n} y_i}{n},
\]
\[
S_y = \sum_{i=1}^{n} x_i y_i - \frac{\sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n}, \quad S_{ss} = \sum_{i=1}^{n} x_i^2 - \frac{\left(\sum_{i=1}^{n} x_i\right)^2}{n}.
\]

where \( \bar{x} \) is the mean of \( x \), \( \bar{y} \) is the mean of \( y \), \( S_y \) is the total sum of squares for \( x \) and \( S_{ss} \) is the sum of products of \( x \) and \( y \).

### 3.2. Non-linear Least-Squares method

The Gauss-Newton method is the iterative method used for solving the non-linear Least-Squares problem such as Monod model for microalgae growth. The general non-linear Least-Squares function is expressed as [10]

\[
\min_x f_i(x) = \frac{1}{2} \left\| r_i(x) \right\|^2_2.
\]

where \( \left\| r_i(x) \right\|_2 \) is the Euclidean norm of \( r_i(x) \) [11].

Since the objective function for Least-Squares is to minimize the \( SSE \), therefore the non-linear Least-Squares function for microalgae growth of Monod model is defined as

\[
\min_{\mu_{max}, K_i} f_i(\mu_{max}, K_i) = \frac{1}{2} \left\| r_i - \frac{\mu_{max} I_i}{K_i + I_i} \right\|^2_2.
\]

The Jacobian of \( f_i(\mu_{max}, K_i) \) is written as

\[
J(\mu_{max}, K_i) = \begin{pmatrix}
\frac{\partial f_i}{\partial \mu_{max}} \\
\frac{\partial f_i}{\partial K_i}
\end{pmatrix}.
\]

The Gauss Newton formula is [12]

\[
J(x)^T J(x) p = -J(x)^T r(x),
\]

where

\[
p = -[J(x)^T J(x)]^{-1} J(x)^T r(x).
\]

If \( r(x) \) approximate to zero then \( p \) will also approximate to zero and can be neglected.

The updated parameter value for \( \mu_{max} \) and \( K_i \) can be calculated by using the equation

\[
x_{i+1} = x_i + p_i,
\]

where \( x \) is a vector form of \( [\mu_{max}, K_i] \).

### 4. Parameter estimation for Monod model

The parameters value of kinetics Monod model for microalgae were estimated by utilizing two Least-Squares methods which are linear and non-linear methods. The \( SSE \) was calculated in order to compare the accuracy of the estimated parameters value.
4.1 Linear Least-Squares regression method

An analytical method for linear Least-Squares estimation of the microalgae growth model was introduced and discussed. Originally, Monod equation is in the form of non-linear and it can be transformed into a linear equation form through the following reciprocal of Monod equation and solved by the linear Least-Squares method [13]

\[
\frac{1}{\mu} = \frac{K_I}{\mu_{\text{max}}} \frac{1}{I} + \frac{1}{\mu_{\text{max}}}. \tag{16}
\]

According to the simple Least-Squares regression line as in Equation (4), thus we obtain

\[
\hat{y} = \frac{1}{\mu}, \quad b = \frac{K_I}{\mu_{\text{max}}}, \quad x = \frac{1}{I}, \quad a = \frac{1}{\mu_{\text{max}}}. \tag{17}
\]

By taking relationships in Equation (16), we acquire the parameter \(\mu_{\text{max}}\) and \(K_I\) as

\[
\mu_{\text{max}} = \frac{1}{a} \quad \text{and} \quad K_I = \frac{b}{a}. \tag{18}
\]

Firstly, the value of \(S_x\) and \(S_y\) were calculated to obtain the value of \(b\) by using Equation (7). After that, we calculate the value of \(\bar{x}\) and \(\bar{y}\) in order to obtain the value of \(a\). The estimated parameters of Monod model shown in Table 1 were obtained by substituting the value of \(a\) and \(b\) into Equation (18).

| Table 1. Estimated parameter value by linear Least-Squares method |
|------------------|------------------|
| \(a\)            | 1.122408         |
| \(b\)            | 3.635328         |
| \(\mu_{\text{max}}\) | 0.890941         |
| \(K_I\)          | 3.238864         |

Meanwhile, the estimated \(\frac{1}{\mu}\) was calculated by substituting the estimated \(\mu_{\text{max}}\) and \(K_I\) into Equation (16) in order to determine the square error between experimental data \(\frac{1}{\mu}\) and estimated \(\frac{1}{\mu}\), and finally the \(SSE\) can be obtained as shown in Table 2.
Table 2. Estimated $\frac{1}{\mu}$ and SSE

| $\frac{1}{\mu}$ | Estimated $\frac{1}{\mu}$ | Square Error |
|-----------------|---------------------------|--------------|
| 2.427184        | 2.468826                  | 0.001734     |
| 2.169197        | 1.197209                  | 0.944761     |
| 1.042753        | 1.160877                  | 0.013953     |
| 0.974659        | 1.143064                  | 0.028360     |
| 0.765111        | 1.137369                  | 0.138576     |
| 0.862069        | 1.133628                  | 0.073745     |

$\text{SSE} = 1.201129$

Graph of $\frac{1}{\mu}$ versus $\frac{1}{I}$ for microalgae growth model as shown in Figure 1 was plotted in order to indicate the linear specific growth rate of the microalgae *Botryococcus Braunii* sp. A best fit line of $\frac{1}{\mu} = 3.635 \frac{1}{I} + 1.122$ is a straight line that represents the experimental data on a scatter plot. From Figure 1, it is clearly shown that the relationship between reciprocal of the specific growth rate and light intensity is linear. The estimated parameter values for microalgae growth model which were shown in Table 1 are lack of accuracy because the $\text{SSE}$ is considered quite large. Hence, the estimated parameter values obtained are considered far from the actual parameters. Under this circumstance, the linear transformation is no longer providing accurate estimates of the parameter. Thus, the most appropriate resolution is achieved by non-linear Least Squares method.

![Figure 1](image_url)

*Figure 1. Linear specific growth rate for microalgae *Botryococcus Braunii* sp*
4.2 Nonlinear Least-Squares method

The estimated parameter in microalgae growth model was obtained by implementing Gauss-Newton method. The initial parameters value for $\mu_{\text{max}}$ and $K_i$ are both chosen as 1. Initial parameters value should be reasonably close to the actual value of the parameter for prevention of large number of iteration. Besides that, the $SSE$ is minimized through iteration process. The estimated parameters value for maximum specific growth rate, $\mu_{\text{max}}$ and saturation constant for light intensity, $K_i$ were shown in Table 3.

| $i$ | $\mu_{\text{max}}$ | $K_i$ | $\left\| \mu_i - \frac{\mu_{\text{max}}I_i}{K_i + I_i} \right\|_2$ |
|-----|-------------------|-------|---------------------------------|
| 0   | 1.000000          | 1.000000 | 0.703886                        |
| 1   | 1.015309          | 2.879044 | 0.609111                        |
| 2   | 1.037327          | 4.872861 | 0.581490                        |
| 3   | 1.060439          | 7.073609 | 0.567757                        |
| 4   | 1.090499          | 10.236845 | 0.553655                       |
| 5   | 1.144439          | 16.534261 | 0.527924                       |
| 6   | 1.258471          | 31.314595 | 0.478653                       |
| 7   | 1.417944          | 54.611697 | 0.440233                       |
| 8   | 1.512041          | 70.129956 | 0.433263                       |
| 9   | 1.531854          | 73.638981 | 0.433033                       |
| 10  | 1.533117          | 73.861392 | 0.433032                       |

The minimum $SSE$ was obtained at $10^{4}$ iteration,

$$SSE = \left\| \mu_0 - \frac{\mu_{\text{max}}I_{10}}{K_{10} + I_{10}} \right\|_2^2 = 0.187517. \quad (19)$$

Since the $SSE$ which shown in Equation (19) is considered as small, thus the estimated value of parameters for non-linear Least Squares are approximate to the actual parameters of microalgae growth model. From Figure 2, it is clearly depicted that the points fall fairly close to the best fit line. Therefore, we can conclude that the line of non-linear growth rate is the best fit to the experimental data of specific growth rate of microalgae Botryococcus Braunii sp. Hence, the estimated parameters shown in Table 3 are the optimal parameters of Monod model of the microalgae.
5. Conclusion and recommendation

In conclusion, the estimated parameters for microalgae Botryococcus Braunii sp growth model were obtained by linear and non-linear least square methods. The non-linear Least-Squares method are more accurate compared to the linear Least-Squares method since the SSE for non-linear Least-Squares is less than the SSE for linear Least-Squares and the non-linear Least-Squares shows a best fit of experimental data.

The Least-Squares method is one of the mathematical methods that find the best fit line for a dataset and providing a visual demonstration of relationship between experimental data. Each point of experimental data is representative of the relationship between two dependent and independent variable such as specific growth rate of microalgae Botryococcus Braunii sp and light intensity. Besides that, prediction of specific growth of microalgae depends on the parameters of Monod equation. Thus, the accuracy of prediction was depending on the accuracy of the parameter estimation. The optimal parameter can be obtained by minimizing the SSE approximates to zero by the Least Squares method. Finally, this study concludes that Least-Squares method is one of the useful mathematical method to estimate the parameters value and predict the behaviour of microalgae growth.

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