Linearized Curve Fitting vs Nonlinear Curve Fitting

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Curve Fitting

Curve Fitting is procedure in which a mathematical formula (equation) is used to best fit a given set of data points. It is also defined as the trend in the data by assigning a single function across the entire range. Linear Curve Fitting uses a straight line function. A straight line is described generally by

$$f(x) = Ax + b$$

The goal is to identify the coefficients A and b such that the function f(x) fits the data well [1]. This paper tries to show how we can fit a function to a given data set either by Linearized Curve Fitting or Nonlinear Curve Fitting. In this paper, we will use the Michaelis-Menten equation.

Michaelis-Menten equation describes the chemical kinetics of enzyme reactions. According to this equation, if v_0 is the initial velocity, v_{max}, the maximum velocity, K_m is the Michaelis constant, and C is the substrate concentration, then $v_0 = \frac{v_{max}}{1+\frac{K_m}{C}}$.

In a typical experiment, v_0 is measured as C is varied, and then v_{max} and K_m are determined from the resulting data using curve fitting.

Table 1.0 Data Set

C	2.5	5.0	10.0	15.0	20.0
v_0	0.024	0.036	0.053	0.060	0.064

Nonlinear Curve Fitting

In most cases, the relationship of the measured values, and variables are nonlinear. Nonlinear curve fitting also tries to find the coefficients that will minimize the deviations from the observed, and expected values.

Gauss-Newton Method

The *Gauss–Newton* method is used to solve non-linear least squares problems. It is a modification of Newton's method for finding a minimum of a function. Unlike Newton's method, the Gauss–Newton algorithm can only be used to minimize a sum of squared function values, but it has the advantage that second derivatives, which can be challenging to compute, are not required.

Using the Gauss-Newton Method, we can determine v_{max} and K_m, from the given data above, and we will get the values

$$(1) \qquad v_{max} = 0.0858573 \text{ and } K_m = 6.5618936,$$

Figure 1.1 shows the data points from Table 1.0 and a curve that shows the best fit of a power function to the data points. It can be observed that the curve fits the general trend of the data but does not exactly match the given data points.

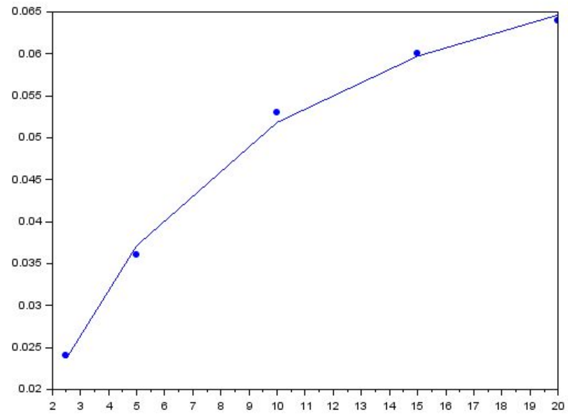

Figure 1.1 Nonlinear Curve Fitting

Linearized Curve Fitting

Alternatively, we can do away with the rigor of nonlinear curve-fitting by rewriting the equation in linear form such as

(i) $1/ v_O = 1/ v_{max} + K_m/ v_{max} \; 1/C$ (Lineweaver)

(ii) $C/ v_O = K_m/ v_{max} + 1/ v_{max} \, C$ (Dixon)

(iii) $v_O = v_{max} - K_m \, v_O/C$ (Eadie)

Linear least-squares

We can find the least squares line by minimizing the sums of squares of the residuals in the transformed equation. Using the same data, determine vmax and Km using linear least squares regression from each of these forms and we shall compare the results with those obtained using nonlinear least squares.

For (i) $1/ v_O = 1/ v_{max} + K_m/ v_{max} \; 1/C$ (Lineweaver) , we get the values $v_{max} = 11.800337$ and $K_m = 75.431449$,

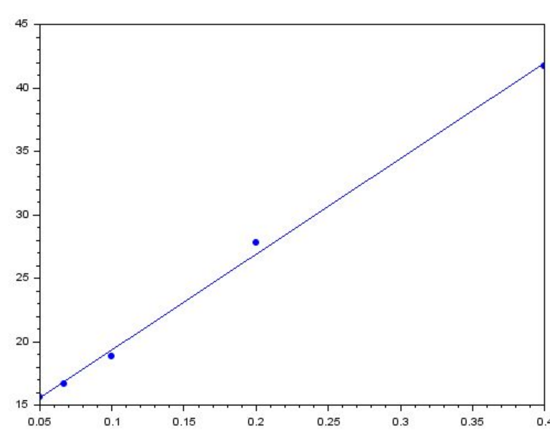

Figure 1.2

For (ii) C/ vO = Km/ vmax + 1/ vmax C (Dixon), we get the values $v_{max} = 75.808055$ and $K_m = 11.717991$,

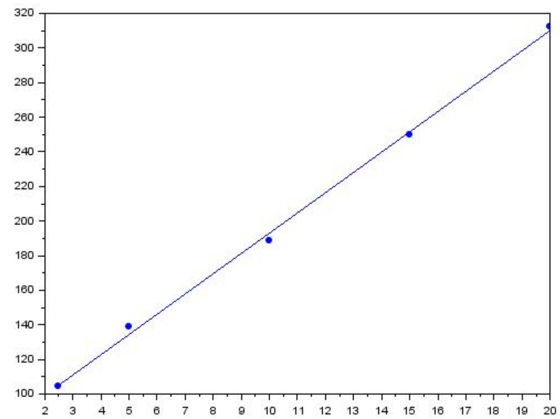

Figure 1.3

For (iii) vO = vmax − Km vO/C (Eadie) , we get the values $v_{max} = 0.0855807$ and $K_m =- 6.5154701$,

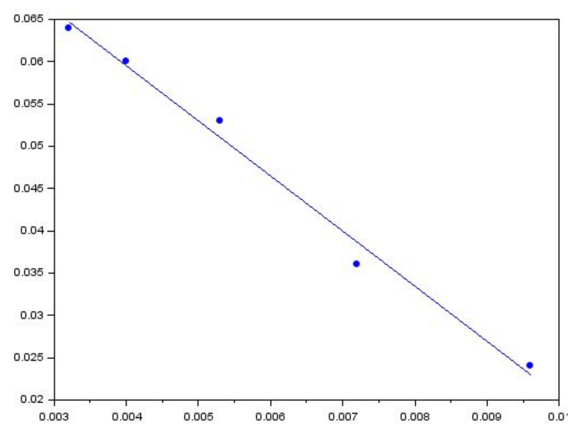

Figure 1.4

We can see that the value nearest to the v_{max} value from (1) is the v_{max} value from Equation (iii), meanwhile the value nearest to the K_m evaluation in (1) is the K_m value from equation (ii).
The Lineweaver-Burk plot, makes use of the double reciprocal plots, which is susceptible to error and tends to concentrate data points into a small region (take a look at Figure 1.2), which are often the least accurate. The double reciprocal plot distorts the error structure of the data, and it is therefore unreliable in determining the kinetic parameters. On the other hand, Eadie-Hofstee plot is a more accurate linear plotting method when v is plotted against v/[S]

References

[1] https://www.essie.ufl.edu/~kgurl/Classes/Lect3421/Fall_01/NM5_curve_f01.pdf
[2] http://physik.uibk.ac.at/hephy/muon/origin_curve_fitting_primer.pdf
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[5] “Numerical Methods for Engineers and Scientists” 3rd Edition. A. Gilat, V. Subramaniam [online] Accessed at