COMMUNICATIONS TO THE EDITOR

A Geometrical Approach for Differentation of an Experimental Function at a Point: Applied to Growth and Product Formation

INTRODUCTION

During studies on fermentation kinetics, the estimation of the parameters of various models[1–5] requires the values of the derivative on the cell mass concentration $[dC(t)/dt]\ t = ti$ or on the production concentration $[dP(t)/dt]\ t = ti$. Unfortunately, $C(t)$ and $P(t)$ are unknown functions and they are available only as a set of experimental data collected during the progress of the fermentation. A rapid and accurate method for the calculation of the derivative of an experimental function at one point based on analytical geometry is developed. The method is compared to graphical and semigraphical procedures for differentiation of experimental functions at a point.

ANALYSIS

Growth and production rates and the rates of utilization of substrates in fermentation processes are often estimated by graphical methods for differentiation. Graphical solutions are good but can vary considerably depending on the investigator's preferences and skills in drawing tangential lines. To obviate these difficulties, the problem was approached through analytical geometry and a computer program developed for making calculations. For development of this theory it is important to assume that there exists an arc of circle $y(x)$ passing through any three points $A(x_A,y_A)$, $B(x_B,y_B)$, and $C(x_C,y_C)$. Under these conditions,

$$\left.\frac{dy(x)}{dx}\right|_{x_B} = \text{slope of the tangent at } B \tag{1}$$

The equations for the straight lines AB and BC are

AB:

$$y = m_{AB}x + n_{AB} \tag{2}$$

with the slope,

$$m_{AB} = \frac{y_B - y_A}{x_B - x_A} \tag{3}$$

and the intercept,

$$n_{AB} = \frac{y_A x_B - y_B x_A}{x_B - x_A} \tag{4}$$

BC:

$$y = m_{BC}x + n_{BC} \tag{5}$$

with the slope,

$$m_{BC} = \frac{y_C - y_B}{x_C - x_B} \tag{6}$$

and the intercept,

$$n_{BC} = \frac{y_B x_C - y_C x_B}{x_C - x_B} \tag{7}$$

Let $M(x_M,y_M)$ and $N(x_N,y_N)$ be the midpoints of AB and BC, straight lines MO and NO should be drawn perpendicular respectively with AB and BC at their midpoints. The equations for MO and NO are, respectively,

MO:

$$y = m_{MO}x + n_{MO} \tag{8}$$

with the slope,

$$m_{MO} = \frac{1}{m_{AB}} = \frac{x_A - x_B}{y_B - y_A} \tag{9}$$

and the intercept,

$$\begin{aligned} m_{MO} &= y_M - m_{MO}x_M \\ &= \left[\frac{y_A + y_B}{2}\right] - m_{MO}\left[\frac{x_A + x_B}{2}\right] \end{aligned} \tag{10}$$

NO:

$$y = m_{NO}x + n_{NO} \tag{11}$$

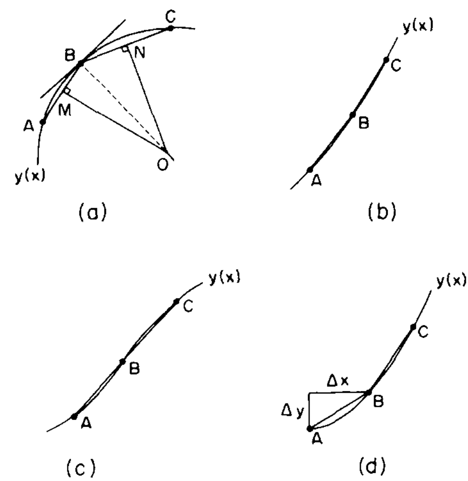

Fig. 1. Illustration for the geometrical differentiation method at point B in the general case (a), when B is on the straight line (b), when B is a point of inflection (c), or at starting point A (d).

with the slope,

$$m_{NO} = -\frac{1}{m_{BC}} = \frac{x_B - x_C}{y_C - y_B} \tag{12}$$

and the intercept,

$$\begin{aligned} n_{NO} &= y_N - m_{NO}x_N \\ &= \left[\frac{y_B + y_C}{2}\right] - m_{NO}\left[\frac{x_B + x_C}{2}\right] \end{aligned} \tag{13}$$

The coordinates of the intersection of these two perpendicular lines at point O (x_O, y_O) are determined by equating eqs. (8) and (11), and hence,

$$x_O = \frac{n_{NO} - n_{MO}}{m_{MO} - m_{NO}} \tag{14}$$

$$y_O = m_{MO}x_O + n_{MO} = m_{NO}x_O + n_{NO} \tag{15}$$

TABLE I

Listing of Subroutine DERIV

```
C
C
      SUBROUTINE DERIV(TETA,CX,DCX,N)
C
C     TETA  = INDEPENDENT VARIABLE
C     CX    = DEPENDENT VARIABLE
C     DCX   = DERIVATIVE OF DEPENDENT VARIABLE
C     N     = NUMBER OF EXPERIMENTAL POINTS (MAXIMUM OF 50)
C
      DIMENSION TETA(50),CX(50),ZMAB(50),ZMBC(50),DCX(50),
     1ZMNO(50),ZNNO(50),ZMMO(50),ZNMO(50),TETAC (50),CXCR(50)
      I = 1
      DCX(I) = (CX(I+1)-CX(I))/(TETA(I+1)-TETA(I))
 0020 ZMAB(I+1) = (CX(I+1)-CX(I))/(TETA(I+1)-TETA(I))
      ZMBC(I+1) = (CX(I+2)-CX(I+1))/(TETA(I+2)-TETA(I+1))
      IF (ABS(ZMAB(I+1)-ZMBC(I+1))-0.001) 0030,0030,0070
 0030 DCX(I+1) = 0.5*(ZMAB(I+1)+ZMBC(I+1))
 0036 I = I + 1
      IF (I-N+2) 0060,0060,0065
 0060 GO TO 0020
 0065 IF (I-N) 0080,0090,0090
 0070 ZMNO(I+1) = (TETA(I+1)-TETA(I+2))/(CX(I+2)-CX(I+1))
      ZNNO(I+1) = 0.5*(CX(I+1)+CX(I+2))-ZMNO(I+1)*0.5*(TETA(I+
     1)+TETA(I+2))
      ZMMO(I+1) = (TETA(I)-TETA(I+1))/(CX(I+1)-CX(I))
      ZNMO(I+1) = 0.5*(CX(I)+CX(I+1))-ZMMO(I+1)*0.5*(TETA(I)+
     1TETA(I+1))
      TETAC (I+1) = (ZNNO(I+1)-ZNMO(I+1))/(ZMMO(I+1)-ZMNO(I+1))
      CXCR(I+1) = ZMMO(I+1)*TETAC (I+1)+ZNMO(I+1)
      DCX(I+1) = (TETAC (I+1)-TETA(I+1))/(CX(I+1)-CXCR(I+1))
      GO TO 0036
 0080 DCX(I+1) = (CX(I+1)-CX(I))/(TETA(I+1)-TETA(I))
      GO TO 0036
 0090 RETURN
      END
```

The equation of the straight line OB is

$$y = m_{OB}x + n_{OB} \tag{16}$$

which has a corresponding slope of

$$m_{OB} = \frac{y_B - y_O}{x_B - x_O} \tag{17}$$

and finally, the slope of the tangent of $y(x)$ at point B is,

$$\left.\frac{dy(x)}{dx}\right|_{x_B} = -\frac{1}{m_{OB}} = \frac{x_O - x_B}{y_B - y_O} \tag{18}$$

The particular cases to be considered are the following. If the slopes of AB and BC are approximately equal (Fig. 1b) where $m_{AB} \cong m_{BC}$, the approximation used is,

$$\left.\frac{dy(x)}{dx}\right|_{x_B} \cong \frac{m_{AB} + m_{BC}}{2} \tag{19}$$

If B is a point of inflection (Fig. 1c), the approximation by eq. (19) may also be

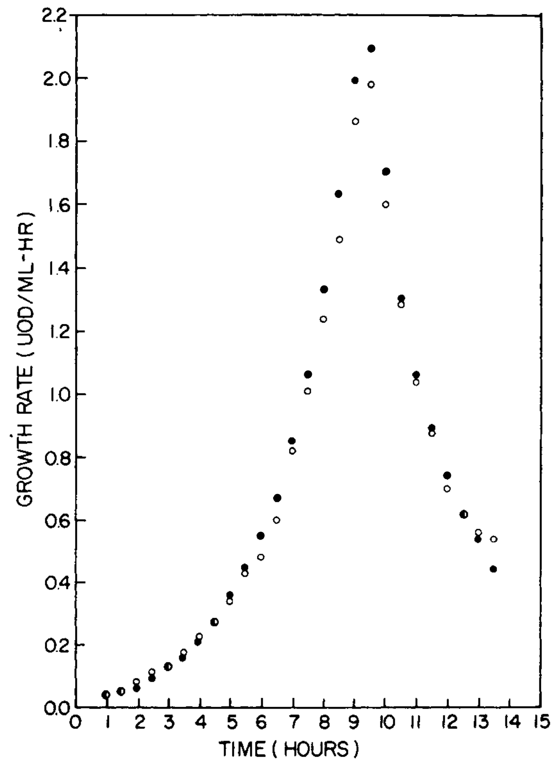

Fig. 2. Comparison of the growth rate obtained by the geometrical method (○) and by the graphical method[2] (●).

used. For the case of either starting point or end point (Fig. 1d), the derivative may be approximated by (only starting point shown):

$$\left.\frac{dy(x)}{dx}\right|_{x_A} \cong \frac{\Delta_y}{\Delta_x} \tag{20}$$

The calculation of eqs. (18), (19), and (20) from a set of experimental data (x_i, y_i) may be performed on a digital computer. For convenience the program written in FORTRAN language under the form of a subroutine, DERIV, is shown in Table I.

EXAMPLES

The subroutine DERIV was used to calculate the growth rate (Fig. 2) and the production rate (Fig. 3) from the experimental data reported by Luedeking and Piret.[2] The results are shown together with those obtained by these authors who used a graphical differentiation method. The values of the derivative obtained from the two methods fitted very closely, except in the vicinity of their maximum values, where the geometrical derivatives are lower (~5%) than the graphical derivatives. In this sensible region, greater error would be expected from the graphical differentiation method. Under this condition, the method shown herein would be far more accurate.

The subroutine DERIV was also used to calculate the derivative of water density with temperature (Fig. 4) from the experimental data[6] which were compared with the results obtained by the semigraphical differentiation method. The results were perfectly fitted, except the end point and the starting point. In general, one would expect to encounter some difficulties in the estimation of the derivative at the end point and the starting point by any method used.

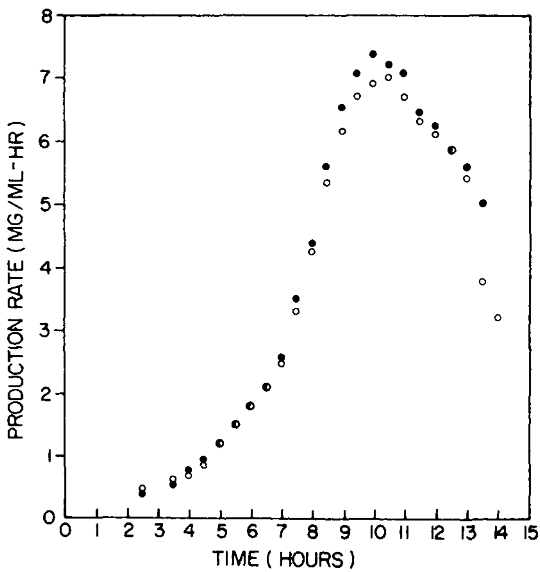

Fig. 3. Comparison of the production rate obtained by the geometrical method (○) and by the graphical method[2] (●).

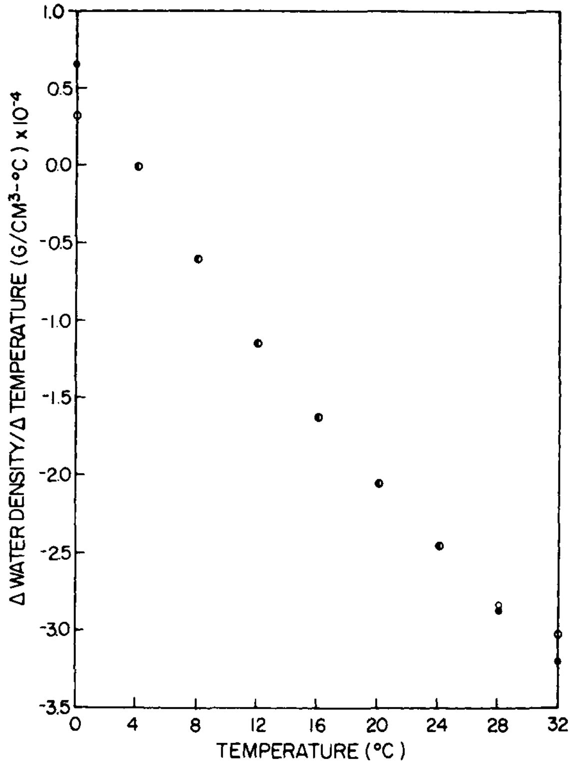

Fig. 4. Comparison of the rate of change of water density with temperature by the geometrical method (○) and by the semigraphical method[6] (●).

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