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TECHNICAL MEMORANDUM 23

CURVE-FITTING GUIDE

NOVEMBER 1962

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BIOLOGICAL LABORATORIES
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U.S. ARMY CHEMICAL-BIOLOGICAL-RADIOLOGICAL AGENCY
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DIRECTOR OF TECHNICAL SERVICES

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ABSTRACT

Various mathematical expressions that may be used to represent experimental data are presented. Specific methods of linear transformation and the general least-squares procedure for functions having nonlinear parameters are described in detail. In addition, brief discussions are given for the following classes of functions: linear combinations of exponentials, asymptotic regression, frequency functions, and polynomials. References are provided that describe the methodology in greater detail.

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TABLE

I. INTRODUCTION

In the analysis of experimental data, it is often desirable to obtain a mathematical expression of the relationship between two variables. The determination of an empirical formula, whose curve will be an appropriate fit for the plotted data, depends upon an understanding of the physical significance of the data and a knowledge of the general nature of a wide variety of curves. Once the equation of a curve has been selected for a set of data, the constants of the equation must be determined by one of the methods available for fitting a curve to experimental data.

The objective of this paper is to present in as concise a form as possible methods for handling a wide variety of functions. The methods discussed here represent the author's investigation into various techniques of curve fitting. Although the investigation has by no means been exhaustive, it is hoped that this collection will serve at least to hasten the work of others who wish to apply the methods of curve fitting, by providing them with a summary of the available straightforward methods, and by directing them to some of the literature available on the treatment of more complex curves. In the interest of keeping the paper brief and easy to follow, proofs and numerical examples of the methods discussed have been omitted. It is recommended that the reader refer directly to the literature for further details on the method he finally decides to employ.

II. STRAIGHT-LINE TRANSFORMATIONS

A. INTRODUCTION

If the experimental data, when plotted on arithmetic coordinate paper, do not approximate a straight line $y = a + bx$ but do seem to approximate a smooth curve, the shape of the curve and an understanding of the nature of the experiment may suggest the equation of the curve that will fit the points most closely. A very helpful way of verifying the appropriateness of a particular equation for a set of data is to transform the data in such a way that a straight-line plot $y' = a' + bx'$ is obtained. If a straight line is achieved through some transformation, the equation corresponding to the transformation will be known to be satisfactory and, furthermore, the parameters of the equation can be evaluated directly from the linear form of the equation.

Table I is furnished as a quick reference to the methods of straight-line transformation available for fitting curves to experimental data. A collection of graphs (Figure 1) is included to illustrate the effect of variation of the parameters (constants) in the equations presented in the table. The general techniques of linear transformation displayed in the table are outlined in Section II. For numerical examples and more detailed explanations of the methods of transformation, the reader is directed to the Literature Cited.[1-8] Johnson[1] treats the widest variety of general types of equations, and his book would be recommended as a first reference. The other books treat much of the same material as Johnson does, but Davis[2] and Running[3] present, in addition, a few of the more specialized procedures that are given in Table I.

B. GENERAL PROCEDURES FOR LINEAR TRANSFORMATION

1. Reciprocals or Logarithms [Equations (1), (2), (3), (4), and (5) of Table I]

Logarithms or reciprocals of one or both of the variables may be taken before the values are plotted on arithmetic coordinate paper. Alternatively, logarithmic or reciprocal paper may be used to eliminate the need for making these additional calculations.

2. Selection of a Point on the Experimental Curve [Equations (3a), (6), and (7) of Table I]

A particular point (x_1, y_1) on the experimental curve may be used to reduce the original equation to a linear form in two parameters. Occasionally, more than one point is used in this way.

3. Combination of Methods (1) and (2) [Equations (4a), (4b), (5a), (5b), and (6a) of Table I]

4. Combination of Two Simple Curves

(a) Sum of two simple equations, each of which influences a particular portion of the curve (Method 14 of Table I).

When a portion of the data appears to be linear on some type of coordinate paper, whereas the remainder shows a distinct curvature, the linear portion may be fitted by the appropriate formula, and then the deviations of the rest of the data from this straight line may be fitted by a second function. The final equation will be the sum of the two functions, each function being negligible for the portion of the curve where the other function has the most influence.

(b) Sum of two simple equations, both of which exert influence over the entire range of the curve [Equations (10), (11), and (12) of Table I].

Although no portion of the plotted curve is linear on any of the types of coordinate paper, some curves may be represented by a sum of simple equations. In this case, ratios of the successive values of y are plotted on arithmetic coordinate paper to obtain a straight line that will give the values of two of the parameters. The remaining two parameters can then be evaluated from the original equation.

(c) Two separate equations, each valid for a restricted range of the variables.

When it is impossible to represent a set of data by an equation involving few constants, it is sometimes advisable to fit different equations to distinct portions of the curve.[4]

C. DETERMINATION OF THE CONSTANTS

Once the equation has been selected, there are several ways in which the parameters of the curve may be approximated, depending on the degree of accuracy required. Reference will be made later in the paper to the principle of maximum likelihood and the method of moments, which are useful in the estimation of parameters for certain types of functions. The three most common methods of parameter estimation, given in the order of the accuracy afforded, are the method of least squares, the method of averages, and the method of selected points. Since these three methods are fully described in standard textbooks, there is no need to give a detailed explanation of them here. The method of least squares gives the best fit and is generally relied upon for accurate estimates of the parameters. Modern-day computing facilities relieve the problems once imposed by the laborious computations required in the least-squares process. A modification of the method of averages has been reported by Nair and Shrivastava[5]. Their method of group averages can be employed to give greater precision than would be furnished by the method of averages with less arithmetic labor than would be required by the method of least squares.

TABLE I. STRAIGHT-LINE TRANSFORMATIONS

	EQUATION	COORDINATES FOR STRAIGHT LINE, x - axis	y - axis	STRAIGHT-LINE EQUATION	COMMENTS	First (a) Reference
(1)	$\frac{1}{y} = a + bx$	x	$\frac{1}{y}$	$\frac{1}{y} = a + bx$	Asymptotes: $x = \frac{-a}{b}$, $y = o$	[illegible]
(2)	$y = a + \frac{b}{x}$	$\frac{1}{x}$	y	$y = a + \frac{b}{x}$	Asymptotes: $x = o$, $y = a$	[illegible]
(3)	$\frac{x}{y} = a + bx \left(\text{or } y = \frac{x}{a + bx}\right)$	x	$\frac{x}{y}$	$\frac{x}{y} = a + bx$	Asymptotes: $x = \frac{-a}{b}$, $y = \frac{1}{b}$	[illegible]
	or $\frac{1}{y} = \frac{a}{x} + b$	$\frac{1}{x}$	$\frac{1}{y}$	$\frac{1}{y} = b + \frac{a}{x}$		1
(3a)	$y = \frac{x}{a + bx} + c$	x where (x_1, y_1) is any point on the experimental curve	$\frac{x - x_1}{y - y_1}$	$\frac{x - x_1}{y - y_1} = (a + bx_1) + \frac{b}{a}(a + bx_1)x$	Asymptotes: $x = \frac{-a}{b}$, $y = \frac{1}{b} + c$. Same curve as (3) shifted up or down by a distance of c.	1
(4)	$y = ax^b$	$\log x$	$\log y$	$\log y = \log a + b \log x$	If b is +, curve has parabolic shape and passes through origin and (1, a). If b is -, curve has hyperbolic shape, passes through (1, a), asymptotic to x and y axes.	1
(4a)	$y = ax^b + c$	$\log x$	$\log (y - c)$	$\log (y - c) = \log a + b \log x$	First find c by equation $c = \frac{y_1 y_2 - y_3}{y_1 + y_2 - 2y_3}$, where $x_3 = \sqrt{x_1 x_2}$, (x_1, y_1) and (x_2, y_2) being points on experimental curve. For 2 other methods, see Running 3.	1
(4b)	$y = c\ 10^{ax^b}$	$\log x$	$\log (\log y - \log c)$	$\log (\log y - \log c) = \log a + b \log x$	After taking logarithms of the original equation, follow method (4a).	3
(5)	$y = ab^x$ [equivalent forms: $y = ae^{b_2 x}$, $y = 10^{a_1 + b_1 x}$, $y = a\,(10)^{b_1 x}$]	x	$\log y$	$\log y = \log a + x \log b$	Passes through the point (o, a)	1
(5a)	$y = ab^x + c$	x	$\log (y - c)$	$\log (y - c) = \log a + x \log b$	First find c by equation $c = \frac{y_1 y_2 - y_3}{y_1 + y_2 - 2y_3}$, where $x_3 = \frac{x_1 + x_2}{2}$, (x_1, y_1) and (x_2, y_2) being points on experimental curve. For 2 other methods, see Running 3.	1
(5b)	$y = 10^{ab^x} + c$	x	$\log (\log y - c)$	$\log (\log y - c) = \log a + x \log b$	After taking logarithms of the original equation, follow method (5a).	
(6)	$y = a + bx + cx^2$	x where (x_1, y_1) is any point on curve	$\frac{y - y_1}{x - x_1}$	$\frac{y - y_1}{x - x_1} = (b + cx_1) + cx$	After finding b and c by the linear transformation, find a by taking the average of all the values of a found by substituting observed values of x and y into the original equation.	1
	Alternate methods: average x in each interval		$\frac{\Delta y}{\Delta x}$	$\frac{\Delta y}{\Delta x} = b + 2cx$		1
		x	Δy	Applicable only when Δx is constant: $\Delta y = [b\Delta x + c(\Delta x)^2] + (2c\Delta x)x$		2
	Alterations of basic parabola (6)					
(6a)	$\frac{1}{y} = a + bx + cx^2$				After making the appropriate transformation by one of the methods outlined in items (1)-(5), follow the first method outlined in Equation (6).	3
(6b)	$y^2 = a + bx + cx^2$					3
(6c)	$y = a + \frac{b}{x} + \frac{c}{x^2}$					3
(6d)	$y = \frac{x}{a + bx + cx^2}$ or $\frac{x}{y} = a + bx + cx^2$					3
(6e)	$y = 10^a + bx + cx^2$					3
(6f)	$y = a + b \log x + c \log^2 x$					3
(6g)	$y = 10^a + b \log x + c \log^2 x$					

(7) $(x + a)(y + b) = c$	$\bar{X} = x - x_1$ $\quad \bar{Y} = \frac{x - x_1}{y - y_1}$ (x_1, y_1) a point on curve	$\bar{Y} = -\frac{1}{y_1 + b}\bar{X} - \frac{x_1 + a}{y_1 + b}$	After [illegible] determine [illegible] values of c found [illegible] of x and y in the original equation.
(8) $a + bx + cd^x$	1. x $\quad \log \Delta^2 y$ 2. x $\quad y - cd^x$	1. $\log \Delta^2 y = x \log d + \log c (d^{\Delta x} - 1)^2$ 2. $y - cd^x = a + bx$	Δx is the constant difference between x values [illegible] c and d from Equation (1). $\Delta^2 y$ is the second difference of the y values [illegible] the values of c and d found by Equation (1) determine a and b from Equation (2).
(9) $y = a\,10^{\frac{b}{x + c}}$	1. $\bar{X} = \frac{1}{x - x_1}\log\frac{y}{y_1}$, $\quad \bar{Y} = \log\frac{y}{y_1}$ 2. $x + c$ $\quad \log y$	1. $\bar{Y} = -(x_1 + c)\bar{X} + \log a - \log y_1$ 2. $\log y = \frac{b}{x + c} + \log a$	Using the values of a and b found [illegible] Equation (1) determine c from Equation (2).
(10) $y = ae^{cx} + be^{dx}$	1. $\bar{X} = \frac{y_{k+1}}{y_k}$, $\bar{Y} = \frac{y_{k+2}}{y_k}$ 2. $e^{(c - d)x}$, ye^{-dx}	1. $\bar{Y} = (e^{c\,\Delta x} + e^{d\,\Delta x})\bar{X} - e^{(c + d)\Delta x}$ 2. $ye^{-dx} = ae^{(c - d)x} + b$	Δx is constant difference between x values. For this line slope M is +, y intercept B is −. [illegible] Using values of c and d found in Equation [illegible] determine a and b from Equation (2).
(11) $y = e^{ax}(c \cos bx + d \sin bx)$	1. $\bar{X} = \frac{y_{k+1}}{y_k}$, $\bar{Y} = \frac{y_{k+2}}{y_k}$ 2. $\tan bx$, $\frac{y}{e^{ax}\cos bx}$	1. $\bar{Y} = 2(\cos b\,\Delta x)e^{a\,\Delta x}\bar{X} - e^{2a\,\Delta x}$ 2. $\frac{y}{e^{ax}\cos bx} = c + d \tan bx$	Δx is constant difference between x values. For this line $(M^2 + 4B)$ is −. (M is slope, B is y intercept). Using values of a and b found in Equation (1) determine c and d from Equation (2).
(12) $y = ax^c + bx^d$	1. $\bar{X} = \frac{y_{k+1}}{y_k}$, $\bar{Y} = \frac{y_{k+2}}{y_k}$ 2. $x^{(c - d)}$, $\frac{y}{x^d}$	1. $\bar{Y} = (r^c + r^d)\bar{X} - r^{c + d}$ 2. $\frac{y}{x^d} = ax^{(c - d)} + b$	r is constant ratio between x values. Slope M is + [illegible] intercept B is −. $(M^2 + 4B)$ is +. Using values of c and d found in Equation (1), determine a and b from Equation (2).
(13) $y = ax^b c^x$	1. x_k, $\quad \log\frac{y_{k+1}}{y_k}$ 2. $\log x_n$, $\log y_n - x_n \log c$	1. $\log\frac{y_{k+1}}{y_k} = (r - 1)x_k \log c + b \log r$ 2. $\log y_n - x_n \log c = b \log x_n + \log a$	r is constant ratio between x values. Using values of c found in Equation (1), determine a and b from Equation (2).

(14) Specialized Method for Fitting Curves that Deviate from a Straight Line for a Portion of the Data:

	Equation	Specific Comments
(14a)	$y = (a + bx) + cd^x$	Type (8)
(14b)	$y = (a + bx) + cx^d$	
(14c)	$y = kx^x g d^x$	
(14d)	$y = ae^{cx} + be^{dx}$	Type (10)
(14e)	$y = ax^c + bx^d$	Type (12)
(14f)	$y = ax^c + be^{dx}$	
(14g)	$y = \frac{x}{a + bx} + ce^{dx}$	
(14h)	$y = \frac{x}{a + bx} + cx^d$	
(14i)	$y = (a + bx) + \frac{\Delta}{2 \cosh[n(\bar{X} - x)]}$	For "bumped" data $\bar{X}$ is value of x corresponding to maximum deviation of y from straight line y'. $\Delta/2$ is this deviation. n must be determined empirically. See Reference 2.

General Method of Fitting:

1. Test plot as you would for simple curves. On one of the types of coordinate paper, the test plot should fall closely on a straight line for part of the data and fall away from it for the other part.
2. Using the straight-line portion of the test plot, determine its equation by the usual methods of linear transformation (items 1-5 above). Call the equation of the straight line y'.
3. Extend the straight line and compute values of y' that correspond to the x values throughout the entire range of the data.
4. Compute the deviations $\Delta y = \lvert y' - y\rvert$ of the straight line y' from the original data y.
5. Test plot $(x, \Delta y)$ for the portion of the curve that does not fall on the straight line y'.
6. If these data are found to fall on a straight line on one of the types of coordinate paper, determine the equation for Δy by the methods of linear transformation.
7. The equation of the curve that corresponds to the entire range of the data will then be $y = y' + \Delta y$ if the original curve y lies above the straight line y' or $y = y' - \Delta y$ if the original curve y lies below the straight line y'.

$\frac{1}{y} = a + bx$

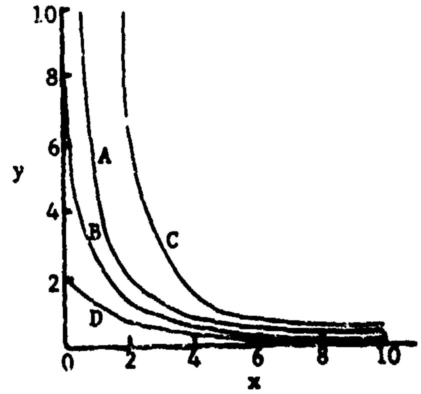
A. $\frac{1}{y} = -.1 + .3x$

B. $\frac{1}{y} = .1 + .3x$

C. $\frac{1}{y} = -.5 + .3x$

D. $\frac{1}{y} = .5 + .3x$

Equation (1)



$y = a + \frac{b}{x}$

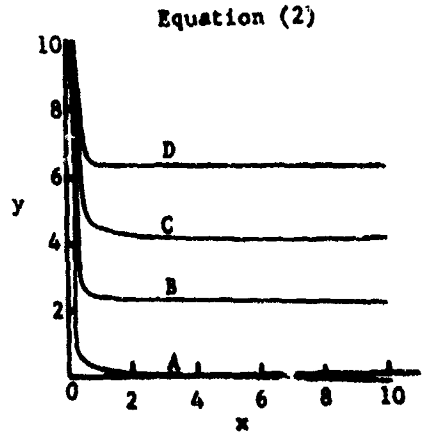
A. $y = -.1 + \frac{.3}{x}$

B. $y = 2 + \frac{.3}{x}$

C. $y = 4 + \frac{.3}{x}$

D. $y = 6 + \frac{.3}{x}$

Equation (2)



$\frac{x}{y} = a + bx$

A. $\frac{x}{y} = -.1 + .3x$

B. $\frac{x}{y} = .1 + .3x$

C. $\frac{x}{y} = -.4 + .3x$

D. $\frac{x}{y} = .4 + .3x$

Equation (3)

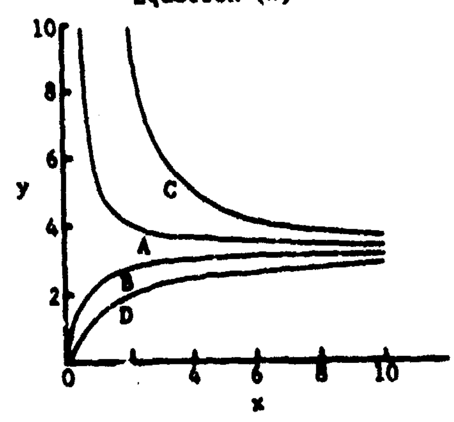


Figure 1. Graphs of Equations (1) through (6), (14b).

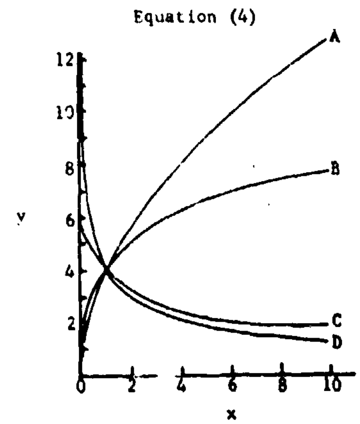
$y = ax^b$

A. $y = 4x^{.5}$

B. $y = 4x^{.3}$

C. $y = 4x^{-.3}$

D. $y = 4x^{-.5}$



$y = ab^x$

A. $y = 2(.2)^x$

B. $y = 2(.3)^x$

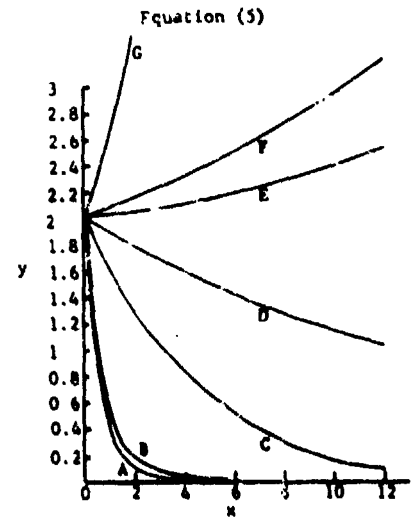
C. $y = 2(.8)^x$

D. $y = 2(.95)^x$

E. $y = 2(1.02)^x$

F. $y = 2(1.04)^x$

G. $y = 2(1.3)^x$



$y = a + bx + cx^2$

A. $y = 1 - .1x + .01x^2$

B. $y = 1 + .1x + .01x^2$

C. $y = 1 - .05x + .005x^2$

D. $y = 1 + .05x + .005x^2$

E. $y = 1 + .05x - .005x^2$

F. $y = .005x + .05x^2$

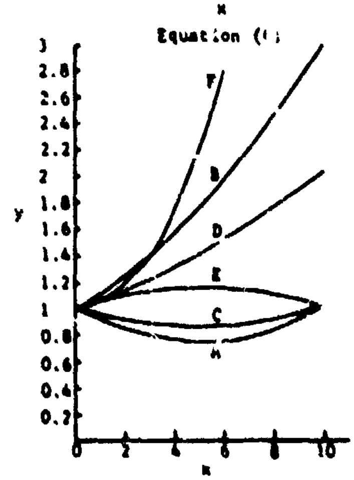


Figure 1. Continued.

$$\frac{1}{y} = a + bx + cx^2$$

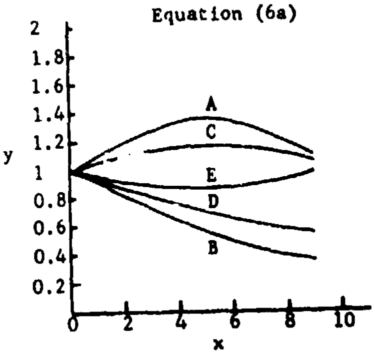
A. $\frac{1}{y} = 1 - .1x + .01x^2$

B. $\frac{1}{y} = 1 + .1x + .01x^2$

C. $\frac{1}{y} = 1 - .05x + .005x^2$

D. $\frac{1}{y} = 1 + .05x + .005x^2$

E. $\frac{1}{y} = 1 + .05x - .005x^2$



$$y^2 = a + bx + cx^2$$

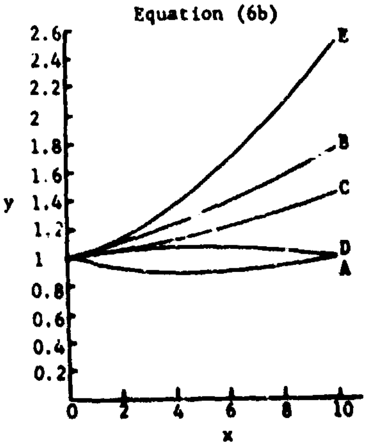
A. $y^2 = 1 - .1x + .01x^2$

B. $y^2 = 1 + .1x + .01x^2$

C. $y^2 = 1 + .05x + .005x^2$

D. $y^2 = 1 + .05x - .005x^2$

E. $y^2 = 1 - .005x + .05x^2$



$$y = a + \frac{b}{x} + \frac{c}{x^2}$$

A. $y = 2 - \frac{2}{x} + \frac{2}{x^2}$

B. $y = 2 + \frac{2}{x} + \frac{2}{x^2}$

C. $y = 2 + \frac{2}{x} - \frac{2}{x^2}$

D. $y = 1 + \frac{1}{x} - \frac{1}{x^2}$

E. $y = .5 - \frac{.2}{x} + \frac{.2}{x^2}$

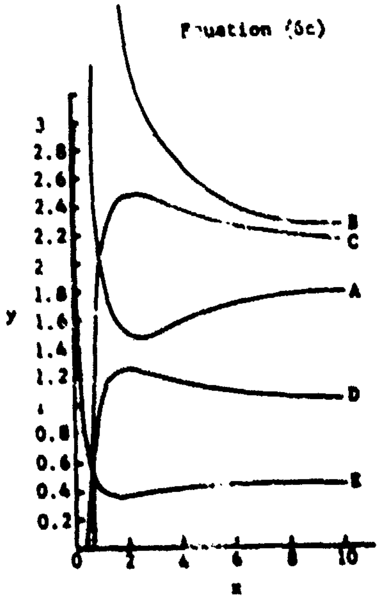


Figure 1. Continued.

$$y = \frac{x}{a + bx + cx^2}$$

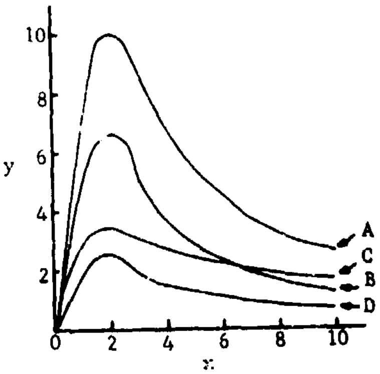
A. $y = \frac{x}{.2 - .1x + .05x^2}$

B. $y = \frac{x}{.3 - .2x + .1x^2}$

C. $y = \frac{x}{.2 + .1x + .05x^2}$

D. $y = \frac{x}{.3 + .2x + .1x^2}$

Equation (6d)



$$y = 10^{a + bx + cx^2}$$

A. $y = 10^{.75 - .30x + .03x^2}$

B. $y = 10^{.375 - .15x + .015x^2}$

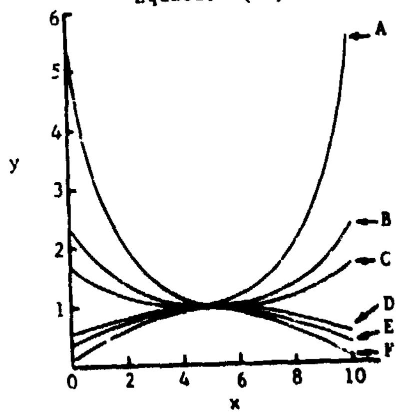
C. $y = 10^{.25 - .10x + .01x^2}$

D. $y = 10^{-.25 + .10x - .01x^2}$

E. $y = 10^{-.375 + .15x - .015x^2}$

F. $y = 10^{-.75 + .30x - .03x^2}$

Equation (6e)



$$y = a + b \log x + c \log^2 x$$

A. $y = 1.2 + \log x + 1.2 \log^2 x$

B. $y = 1.2 + \log x + .12 \log^2 x$

C. $y = 1.2 - \log x + 1.2 \log^2 x$

D. $y = 1.2 - \log x + .12 \log^2 x$

Equation (6f)

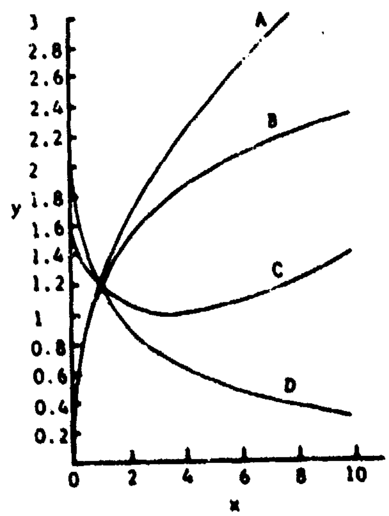


Figure 1. Continued.

$$y = 10^{a + b \log x + c \log^2 x}$$

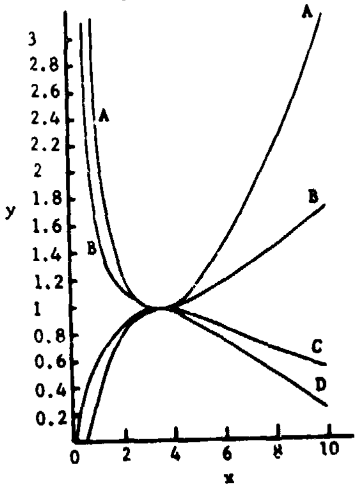
A. $y = 10^{.50 - 2 \log x + 2 \log^2 x}$

B. $y = 10^{.25 - \log x + \log^2 x}$

C. $y = 10^{-.25 + \log x - \log^2 x}$

D. $y = 10^{-.50 + 2 \log x - 2 \log^2 x}$

Equation (6g)



$$y = a + bx + cx^{-d}$$

A. $y = 1 + x + 6x^{-3}$

B. $y = 1 + x + 4x^{-3}$

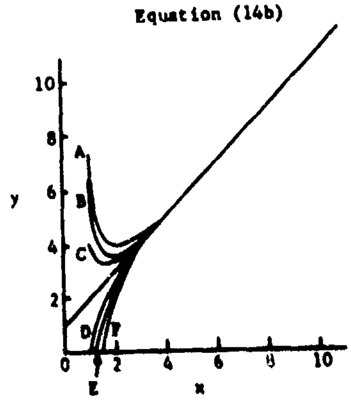
C. $y = 1 + x + 2x^{-3}$

D. $y = 1 + x - 2x^{-3}$

E. $y = 1 + x - 4x^{-3}$

F. $y = 1 + x - 6x^{-3}$

Equation (14b)



$$y = a + bx + cx^{d}$$

A. $y = 1 + x + .001x^4$

B. $y = 1 + x + .0002x^4$

C. $y = 1 + x + .0001x^4$

D. $y = 1 + x - .0001x^4$

E. $y = 1 + x - .0002x^4$

F. $y = 1 + x - .001x^4$

Equation (14b)

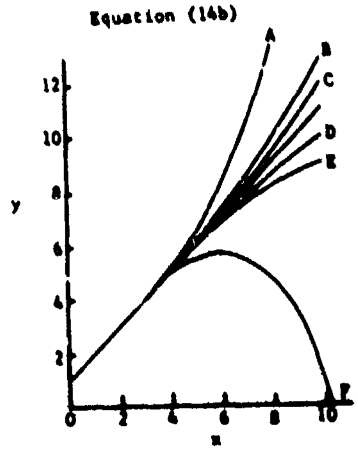


Figure 1. Continued.

The method of selected points, though least accurate, is very simple and can be used to get an immediate rough idea of the nature of the parameters. In employing this method, the straight line is usually fitted manually to the plotted points. The arbitrary eye fit is the main factor contributing to the inaccuracy of this method of estimating the parameters. Askovitz[7] has described a very interesting method of fitting a least-squares straight line to a series of points by a method that is entirely graphical. Since this method is not well known and can considerably improve the accuracy of the method of selected points (provided only that the x values of the points are equally spaced), it will be described briefly in the next section. For proof of the method, the reader should refer to the original work.

D. SHORT-CUT GRAPHIC METHOD FOR FITTING THE BEST STRAIGHT LINE TO A SERIES OF POINTS ACCORDING TO THE CRITERION OF LEAST SQUARES*

Given: Five points — A, B, C, D, E, (or any number of points), with values of x at equal intervals Δx. Consider the value of Δx to be a spacing unit.

Method:

(a) Place straightedge so that it joins A and B (Figure 2). Draw a straight line from A to a point 2/3 of a spacing unit farther. The point found is B'. Note that B' lies on a vertical line 2/3 Δx to the right of A.

(b) Place straightedge so that it joins B' to C. Starting at B', draw a straight line 2/3 of a spacing unit farther. The point found is C', and lies on a vertical line 2/3 Δx to the right of B'.

(c) Continue in this manner. Call the last point found T.

(d) Now start at E and go backwards in the same manner. Call the last point found U.

(e) UT is the line of best fit by least squares for the points A to E.

(f) As a check on the procedure, x values of A, U, T, and E should be found to be equally spaced.

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* "Advancing Centroids Technique" (condensed from a paper by Askovitz[7]).

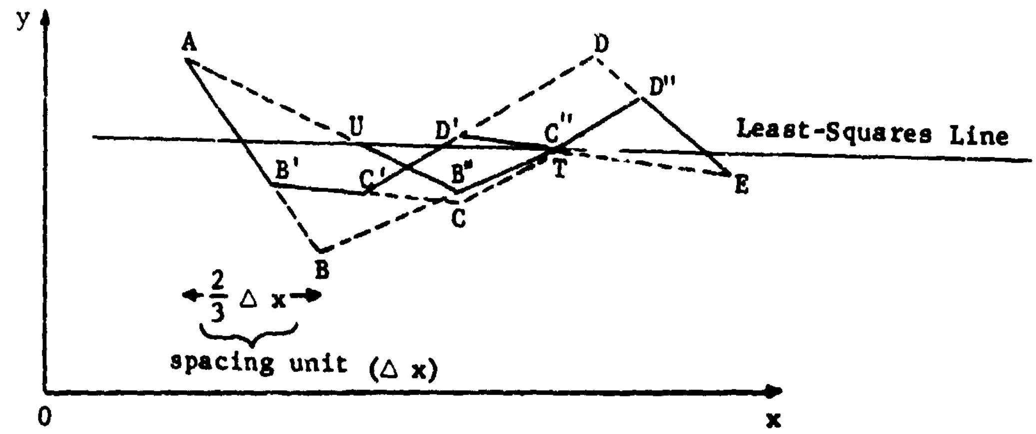


Figure 2. Graphic Method of Fitting Straight Line.

E. EXPLANATION OF TABLE I

For each of the equations stated in the first column of Table I, the second column gives the coordinates that will yield a straight line on arithmetic coordinate paper when the equation is appropriate for the given data. Column 3 gives the corresponding linear equation from which the parameters of the function may be determined. One reference for each method is cited in the last column.

The most common methods of linear transformation are described in items (1) through (5) of Table I. Familiarity with these techniques will assist the reader in understanding the later entries in the table. Item (6) describes a method for transforming a parabola to linear form. A number of variations of the basic equation for a parabola are given in items (6a) through (6g). Once these variations have been reduced to the basic parabola equation by one of the transformations outlined in items (1) through (5), they may be handled by the general method for a parabola as explained in item (6).

Determination of the parameters in Equations (8) through (13) requires the use of two linear equations. The first linear equation yields estimates of two of the parameters, which are used subsequently in the second equation to find the remainder of the parameters. The method presented in item (14) of the table is appropriate only when a portion of the plotted data is linear either immediately or after some transformation has been performed. It should be noted that Equations (8), (10), and (12) may be handled by more general methods when the special condition of partial linearity necessary for Method (14) is not present.

When the symbols Δx and Δy appear in items (6) through (11), they signify the differences between successive values of the data, so that $\Delta x = x_{k+1} - x_k$ and $\Delta y = y_{k+1} - y_k$. The use of the symbol Δy in Method (14) is explained in the table.

A comment is needed concerning Equation (14i) in the table,

$$y = (a + bx) + \frac{\alpha}{2 \cosh [n(\bar{X} - x)]}$$

The final term, $\delta = \dfrac{\alpha}{2 \cosh [n(\bar{X} - x)]}$ which can also be written in the form $\delta = \dfrac{\alpha}{e^{n(\bar{X} - x)} + e^{n(x - \bar{X})}}$, introduces a bump into the curve. The significance of the parameters $\bar{X}$ and α is explained in the table. The effect that this term has when added to equations for a straight line and for a parabola is illustrated in Figures 3 and 4.

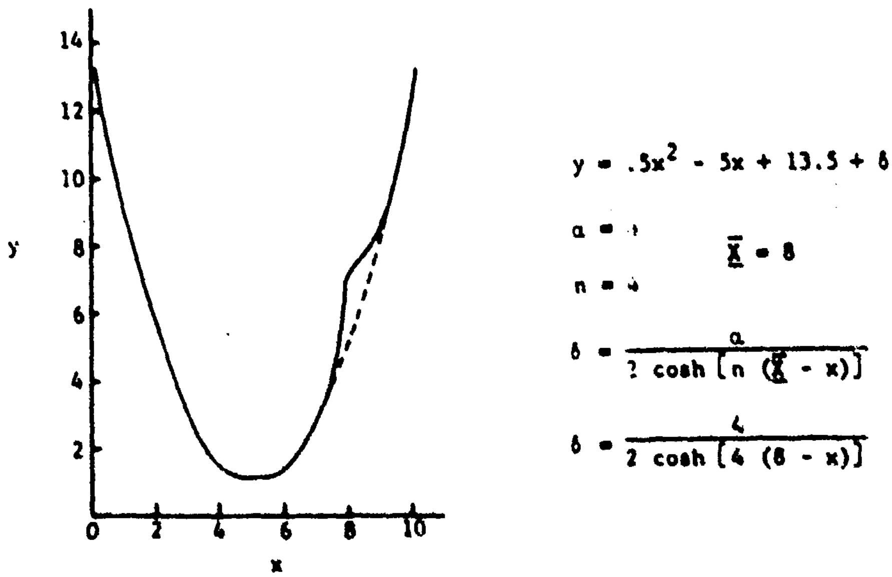


Figure 3. Graph of Variation of Equation (14i).

$$y = a + bx + \delta$$

$$y = 1 + x + \delta$$

$$\delta = \frac{\alpha}{2 \cosh n\,(\bar{X} - x)}$$

$$\bar{X} = 5$$

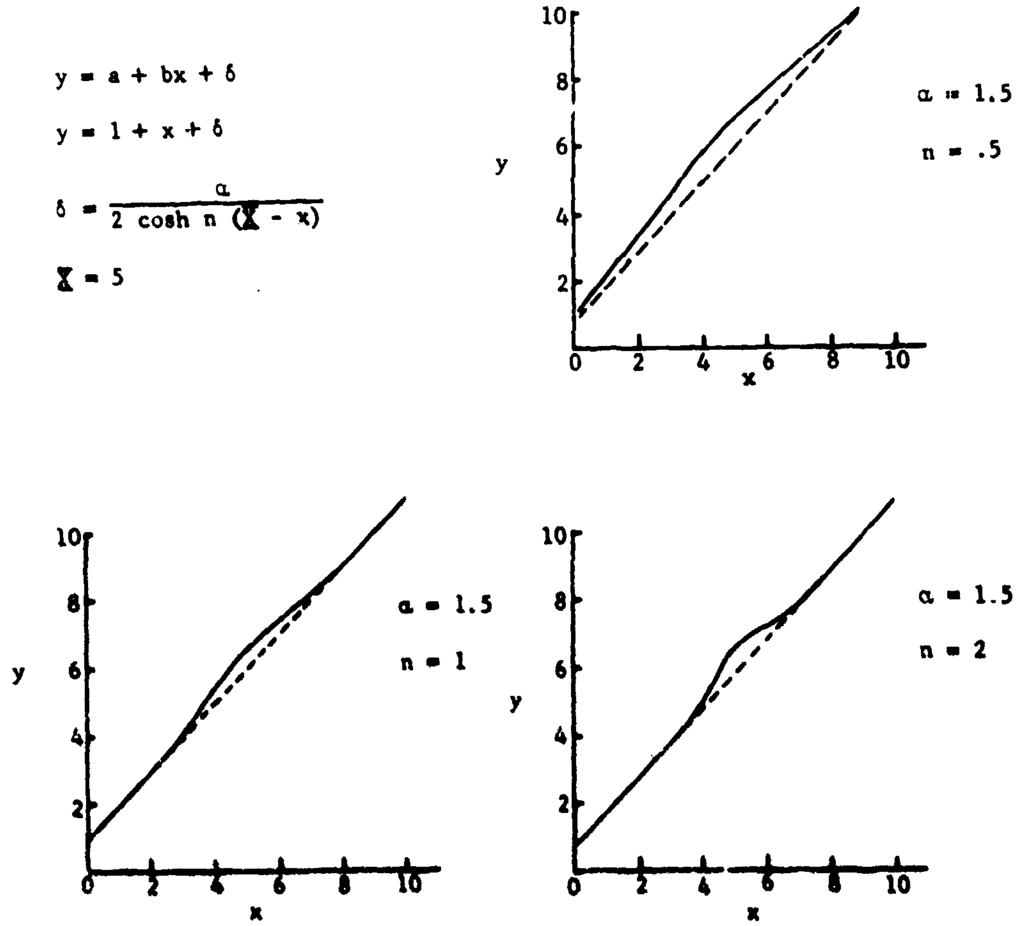


Figure 4. Graphs of Equation (141).

III. METHOD OF DIFFERENTIAL CORRECTION

A. INTRODUCTION

Equations that contain nonlinear parameters, and for which no transformation will afford a linear relation among the parameters, cannot be handled by the usual methods described in Section II. A general method that will handle such formulas is known as the method of differential correction. This method is an iterative process for which initial estimates of the parameters are required. By considering the approximate values of the constants and the corrections to each of these values, the original function can be expanded in a Taylor's series, which will be linear in the corrections when terms of higher order than the first are neglected. Either the method of averages or the method of least squares will then yield the values of the corrections. Addition of the corrections to the starting values will furnish new estimates and the process may be repeated for improved accuracy.

Modern high-speed computers overcome the difficulties once posed by the rather lengthy calculations necessitated by this method. Furthermore, the method of least squares is usually selected for machine solution of the corresponding regression equation because accuracy, rather than ease of computation, is of primary concern. The method of differential correction is, as a result, often referred to as the "general least-squares method for nonlinear parameters."

This iterative procedure has the limitation that the original estimates of the parameters must be close enough to the true values that higher order terms of the Taylor's series may be omitted without affecting the convergence of the procedure. Starting values may often be obtained from a knowledge of the physical characteristics of the problem whose data are being analyzed. Certain graphical techniques analogous to those described in Section II will also be helpful for certain types of data. If an analog computer is available, it can furnish starting values for a wide variety of functions, by minimizing the area between a series of line segments drawn through the data points, and the curves obtained by varying the parameters in the equation selected for representation of the data.

Although the method of differential correction is often reported in the literature, it is not always described in a detailed and notationally simple manner. For the benefit of the reader not familiar with this method, the author has included a summary of the material presented in the references. For straightforward descriptions of the method, the reader may refer to Running[3], Scarborough[8], and Nielson[8]. More theoretical discussions are given by Deming[9] and Guest[10]. Williams[11] and Turner, Monroe, and Lucas[12] employ a modification of the procedure. Specific applications of the process are reported by Howell[13] and Berkson and Gage[14].

B. EXPLANATION OF THE METHOD

Consider a function

$$y = f\ (x;\ a,\ b,\ c), \tag{1}$$

where x and y are the variables, and a, b, and c are the parameters. Let a_o, b_o, c_o be approximate values of a, b, c, and let Δ a, Δ b, Δ c represent corrections to these initial values such that

$$\begin{aligned} a &= a_o + \Delta a \\ b &= b_o + \Delta b \\ c &= c_o + \Delta c. \end{aligned} \tag{2}$$

A first approximation to the true function is

$$y_o = f\ (x;\ a_o,\ b_o,\ c_o). \tag{3}$$

Rewriting Equation (1) in terms of (2) yields

$$y = f\ (x;\ a_o + \Delta a,\ b_o + \Delta b,\ c_o + \Delta c) \tag{4}$$

Equation (4) may be expanded by Taylor's theorem for a function in several variables to obtain

$$y = f\ (x;\ a_o,\ b_o,\ c_o) + \frac{\partial f}{\partial a_o} \Delta a + \frac{\partial f}{\partial b_o} \Delta b + \frac{\partial f}{\partial c_o} \Delta c \tag{5}$$

$$+ \text{ higher order terms in } \Delta a,\ \Delta b,\ \Delta c,$$

where $\frac{\partial f}{\partial a_o}$ means $\frac{\partial f(x;a,b,c)}{\partial a}$ evaluated at $a = a_o$, $b = b_o$ and $c = c_o$.

Neglecting the higher order terms, substituting and transposing y_o, Equation (4) becomes

$$y - y_o = \frac{\partial f}{\partial a_o} \Delta a + \frac{\partial f}{\partial b_o} \Delta b + \frac{\partial f}{\partial c_o} \Delta c \tag{6}$$

which is linear in the corrections Δ a, Δ b, Δ c.

Equation (6) corresponds to the multiple linear-regression equation

$$R = A_o Z_o + A_1 Z_1 + A_2 Z_2 \tag{7}$$

where

$$R = y - y_o$$

$$A_0 = \Delta a \qquad Z_0 = \frac{\partial f}{\partial a_o}$$

$$A_1 = \Delta b \qquad Z_1 = \frac{\partial f}{\partial b_o}$$

$$A_2 = \Delta c \qquad Z_2 = \frac{\partial f}{\partial c_o}$$

This equation may be solved by the usual method of least squares to obtain the values for Δa, Δb, and Δc.

C. MODIFICATION OF THE METHOD

Many functions contain both linear and nonlinear parameters. Turner[13] has reported a modification of the general least-squares method that eliminates the necessity of using any trial values for the linear parameters, thus reducing the amount of work involved in the solution. In Turner's method, the regression equation is taken from Equation (5) without transposing y_o. He has found that the linear parameters may then be computed directly, thus eliminating the terms containing partial derivatives with respect to the linear parameters. For example, if $f(x; a, b, c)$ is a function in which a and b are nonlinear parameters and c is a linear parameter, the regression equation will be

$$y = f(x;\ a_o,\ b_o,\ c) + \frac{\partial f}{\partial a_o}\Delta a + \frac{\partial f}{\partial b_o}\Delta b, \tag{8}$$

where $\frac{\partial f}{\partial a_o}$ and $\frac{\partial f}{\partial b_o}$ are evaluated at a_o and b_o, but c remains variable. This modification considerably simplifies the general method of least squares, by requiring initial estimates of only the nonlinear parameters, and by permitting the direct use of the observed y values, rather than requiring calculation of the residuals $R = y - y_o$.

D. EXAMPLES

Consider the problem of fitting the function

$$f(x;\ a,\ b) = y = ab^x$$

to a set of experimental data. Although this function contains a nonlinear parameter b, the equation does happen to be one of the types for which a linear transformation is available. The regular least-squares procedure for linear parameters, when applied to the linearized data, will supply directly the best estimates of the parameters, and hence would usually be employed for this simple formula. It is interesting, however, to consider the application of the method of differential correction to the estimation of the parameters in this formula. A straight line may be fitted by eye to the linear transformation of the data to obtain starting values a_0 and b_0. By the method of differential correction, we wish to obtain corrections Δa_0 and Δb_0 such that improved estimates will be

$$a_1 = a_0 + \Delta a_0$$

$$b_1 = b_0 + \Delta b_0$$

If a_1 and b_1 still do not meet the requirements for accuracy, they may then be used as estimates to obtain new values for the corrections, and hence improved estimates

$$a_2 = a_1 + \Delta a_1$$

$$b_2 = b_1 + \Delta b_1.$$

The process may be repeated as many times as necessary to obtain the desired precision. The two methods for obtaining the values of the corrections are illustrated below.

Example 1: Fitting $y = ab^x$ by the General Least-Squares Method for Nonlinear Parameters

Given the function

$$f\ (x;\ a,\ b) = y = ab^x, \tag{9}$$

its partial derivatives with respect to the parameters are

$$\frac{\partial f}{\partial a_0} = b_0^x, \qquad \frac{\partial f}{\partial b_0} = a_0\ x\ b_0^{x-1}.$$

Then the linearized equation [Equation (6)] is

$$y - y_0 = b_0^x\ \Delta a + a_0\ x\ b_0^{x-1}\ \Delta b, \tag{10}$$

where

$$y_0 = f\ (x;\ a_0,\ b_0) = a_0\ b_0^x.$$

If we set

$$R = y - y_0$$

$$A_0 = \Delta a \qquad Z_0 = b_0^x$$

$$A_1 = \Delta b \qquad Z_1 = a_0 \, x \, b_0^{x-1}$$

the regression equation becomes

$$R = A_0 Z_0 + A_1 Z_1$$

and may be solved for A_0 and A_1 (i.e., the values of the corrections) by the usual least-squares procedure.

Example 2: Fitting $y = ab^x$ by the Simplified Method for Equations Containing both Linear and Nonlinear Parameters

Again consider Equation (9). Using Turner's method, only the nonlinear parameter b need be assigned a starting value b_0. The linearized equation [comparable to Equation (8)] takes the form

$$y = a\, b_0^x + a\, x\, b_0^{x-1} \Delta b \tag{11}$$

If we set

$$B_0 = a \qquad X_0 = b_0^x$$

$$B_1 = a \Delta b \qquad X_1 = x b_0^{x-1}$$

the regression equation becomes

$$y = B_0 X_0 + B_1 X_1.$$

This equation may be solved by the method of least squares to obtain B_0 and B_1. The value for B_0 yields the value of a, which in turn, can be used with the value of B_1 to solve for Δb.

E. SPEEDING THE CONVERGENCE

In many cases, convergence is slow due to the oscillations of the parameter estimates about the true value. It has been found that these oscillations may be damped by adding only a fractional part of the corrections to the parameter estimates when obtaining new estimates. Then parameter estimates to be used in the next cycle of iteration will be of the form

$$a_1 = a_0 + \theta \Delta a_0$$

$$b_1 = b_0 + \theta \Delta b_0$$

where θ will usually, but not always, be less than one.

Weinstein[15] specifically discusses the use of a multiplier to accelerate convergence. Turner[12], Howell[13], and Will[16] employ such a factor in performing the least-squares iterative procedure. Box[17] describes the Princeton-IBM 704 program, which computes the optimum value of θ before obtaining the parameters of the function by nonlinear least squares.

F. DISCUSSION

It may be noted that the method of differential correction is a generalization of the least-squares process we commonly use for equations involving only linear parameters. This general method, therefore, may be used for any function, whether it contains linear, nonlinear, or a combination of the two types of parameters. In particular, if the general least-squares procedure is applied to an equation having only linear parameters, and the initial estimates a_o, b_o, c_o are each taken to be zero, then the corrections Δ a, Δ b, Δ c arrived at in the solution are simply the values a, b, c of the parameters themselves, so that the general method reduces to the special case we generally employ.

Often the mathematical model for an experiment is written in terms of a differential equation. Such an equation sometimes cannot be integrated explicitly, so that the partial derivatives of the function cannot be obtained by direct differentiation. Box[17] suggests that if small changes are made in each of the parameters in turn, the numerical value of the derivatives may be calculated from the differences.

Unfortunately, there are times when even the use of the θ multiplier does not improve convergence satisfactorily. For additional consideration of the convergence problem, the reader may refer to the paper by Box[17], who has had considerable experience with the nonlinear least-squares process.

IV. LINEAR COMBINATIONS OF EXPONENTIALS

Experimental data are frequently found to be well represented by sums of exponentials of the general form

$$y = \sum_{i=1}^{n} A_i \, e^{-b_i X}$$

As a result, a number of methods for estimation of the parameters of such a function have been investigated and reported in the literature. Some of these methods will be mentioned briefly here. For the details, direct reference should be made to the literature.

Feurzeig and Tyler[18] have illustrated clearly the graphical "peeling off" procedure explained in item (14) of Table I. They have extended the method to the case of an equation containing more than two terms, but the parameter estimates obtained are only approximate. A method developed by Prony and discussed by Whittaker and Robinson[19], Cornell[20], and Cornfield et al[21], can sometimes be used to advantage in obtaining initial estimates for later refinement by one of the iterative procedures. Iterative maximum likelihood techniques, one of which is similar to the iterative least-squares procedure, are briefly reviewed by Cornell[20].

Taylor[22] used difference equations in his method of attacking the problem. The parameter estimates obtained by his process, however, have not been found to be as consistently accurate as those calculated by some of the other methods.

Cornell[20] has developed an effective noniterative procedure for fitting a fairly general class of linear combinations of exponentials to data taken at equally spaced intervals. He derives expressions that employ as many sums of the observations as there are parameters to be estimated. His method has two advantages over the Prony method; it does not place a limit on the number of observations, and it does not require least-squares calculations.

Hartley's "Internal Least Squares"[23] is a fairly well-known method that can be applied to functions having linear differential equations, and hence to linear combinations of exponentials, because they are generated by linear differential equations. The linear difference equation corresponding to the differential equation is integrated numerically. In the resulting regression equation "the dependent variate y is related to its own repeated sums as independent variables."[23] The principle of least squares is then applied to this regression equation.

V. ASYMPTOTIC REGRESSION

A. INTRODUCTION

Curves that asymptotically approach a limit are often appropriate for representation of experimental data. The modified exponential equation $y = \alpha + \beta\rho^x$ has been used widely to express such relationships. This formula is a particularly useful one, because simple transformations will reduce several other equations to the same general form. The logistic, Gompertz, and Mitscherlich equations are common variations, and much study has been devoted to each of these individual curves, as well as to the general modified exponential. Graphs of various forms of the modified exponential are provided in Figures 5, 6, and 7. A comparison of the properties of the various forms of the equation has been made by Croxton and Cowden[24]. They note that, when the x values of the function are equally spaced, the first differences of y change by a constant percentage in the modified exponential, whereas the first differences for the logistic resemble a normal curve, and for Gompertz's law resemble a skewed frequency curve.

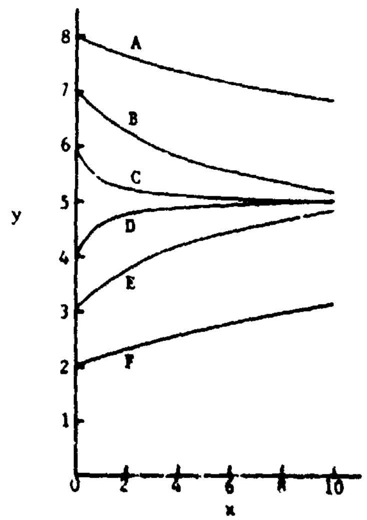
B. ESTIMATION OF THE PARAMETERS

The methods available for estimation of the parameters in an asymptotic regression are numerous. In addition to the general methods for exponentials discussed in Section IV, other methods suitable for functions of the specific form $y = \alpha + \beta\rho^x$ have been reported. Cowden[25] has treated a method of selected points and a graphical method. Nelder's[26] approach is based on internal least squares. Stevens[27] has developed an iterative method and provided tables to facilitate its application. Patterson[28-30] presents formulas for obtaining a fairly accurate estimate of ρ that may be used subsequently as a starting value for Stevens' method or to obtain approximate values of α and β from the linear regression of y on ρ^x.

The form $y = A\left[1-10^{-c(x+b)}\right]$ of the modified exponential is known as Mitscherlich's law. Pimentel-Gomes[31] has applied this form of the equation to a series of experiments on fertilizers. His method of parameter estimation has been used widely and found very acceptable. An extension of Gomes' and Stevens' tables has been provided by Byrd, Jones, et al.[32]

C. GOMPERTZ CURVE

The Gompertz curve, $y = ka^{b^x}$, can be dealt with by the methods already explained if the equation is transformed by logarithms to the form $\log y = \log k + (\log a)\, b^x$. Specific formulas are also available for direct estimation of the parameters from the original form of the Gompertz equation. Kenney[33], Davis[2], and Croxton and Cowden[24] have treated the Gompertz curve in particular, and they have presented appropriate formulas for its solution.



$y = \alpha + \beta\rho^{x}$

A. $y = 5 + 3\,(.95)^{x}$

B. $y = 5 + 2\,(.8)^{x}$

C. $y = 5 + (.3)^{x}$

D. $y = 5 - (.3)^{x}$

E. $y = 5 - 2\,(.8)^{x}$

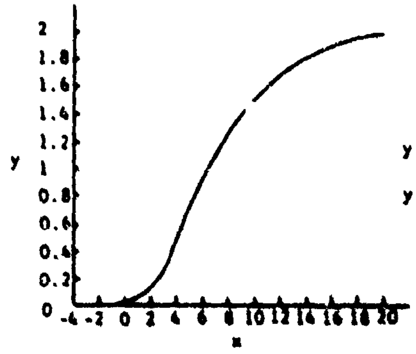
F. $y = 5 - 3\,(.95)^{x}$

Mitscherlich's Form of Equation D

$$y = A\left[1 - 10^{-c\,(x + b)}\right]$$

$$y = 5\left[1 - 10^{-.52284\,(x + 1.33687)}\right]$$

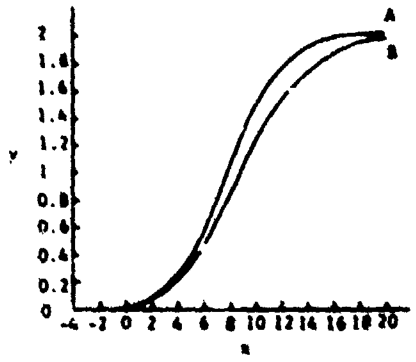
Figure 5. Graph of Modified Exponential Curve.



$y = K\,a^{b^{x}}$

$y = 2\,(.0126)^{0.75^{x}}$

Figure 6. Graph of Gompertz Curve.



Simple Logistic

$$y = \frac{K}{1 + e^{a + bx}}$$

$$\text{A.}\quad y = \frac{2}{1 + e^{4 - .5x}}$$

General Logistic

$$y = \frac{K}{1 + e^{a + bx + cx^{2} + \ldots}}$$

$$\text{B.}\quad y = \frac{2}{1 + e^{4 - .5x + .006x^{2}}}$$

Figure 7. Graph of Logistic Curves.

D. LOGISTIC CURVE

One of the most widely used asymptotic curves is the logistic, whose equation is

$$y = \frac{k}{1+e^{a+bx}}$$

Taking reciprocals will transform the logistic to

$$\frac{1}{y} = \frac{1}{k} + \frac{1}{k} e^{a} (e^{b})^{x}$$

which is, again, a modified exponential. Such a transformation is rarely performed, however, because the methods of dealing with the logistic itself are so numerous.

One of the simplest and best known ways of obtaining parameter estimates is the transformation of the equation into the form

$$\ln \frac{k-y}{y} = a + bx$$

which is a straight line on semi-logarithmic graph paper when x is plotted against (k-y)/y. Pearl[34] and Reed and Berkson[35] have illustrated this method of fitting, and have also given good discussions of the general properties of the logistic function.

Berkson[36-37] has provided graph paper scaled in such a way that the linear relation may be obtained by plotting x directly against y/k. Berkson's "logit paper" is similar to an earlier logistic grid reported by Wilson[38]. Hodges[39] explains a "transfer method which can be used to improve the estimates obtained from the linear plot on logit paper." Berkson[36,40] has also provided tables for the logit and antilogit, to facilitate the determination of the maximum likelihood estimate of the logistic function.

Several other linear transformations of the logistic have been developed. Nair[41] gives a very good summary of five transformations that are based on the differential equation of the logistic or on some form of the corresponding difference equation.

A generalization of the logistic sometimes provides a better fit for a set of experimental data. Terms may be added to the exponential to alter the shape of the curve appropriately. The general logistic is given in the form

$$y = \frac{k}{1 + e^{a+bx+cx^2+\ldots}}$$

where the number of terms in the exponent is determined by the type of fit desired. Figure 7 illustrates the difference between a simple logistic curve and a more general logistic, whose exponential is quadratic. Bailey[42] has published some tables for use in fitting the generalized logistic.

There are many other equations that can be used to represent symmetrical growth curves besides that of the logistic function. Questions often arise as to which equation would be most appropriate for a certain set of data. An interesting article by Winsor[43] compares the logistic with the integrated normal curve, the arc-tangent curve, and the integrated Pearson Type VII curve.

VI. POLYNOMIALS

The use of polynomials in curve fitting is extremely common and easily achieved. The method of least squares yields parameter estimates immediately, because all parameters in the polynomial equation are linear. When the x values of the data are equally spaced, the successive differences of the y values may be examined as an aid in determining the appropriate number of terms for a polynomial that will represent the data adequately[8]. Under this condition, if the n^{th} differences of the y's are constant, then the last term in the required polynomial will be x^n. It is advantageous to use orthogonal polynomial equations when the degree of the polynomial needed to fit the data satisfactorily is not known. Orthogonal polynomials enable higher degree terms to be added to the equation without changing the coefficients of the previously fitted polynomial. Most textbooks describe the technique of using orthogonal polynomials in curve fitting. Paradine and Rivett[44], in particular, give a good exposition of the subject.

Because of the general familiarity with the methods of polynomial regression, polynomials are often overused for curve fitting. In spite of the fact that a polynomial can be found to fit any set of data if a sufficient number of terms are taken, there is often very little biological or physical significance for the parameters of the resulting polynomial. Considerable thought should be given, therefore, to the physical basis of the problem, in order to determine whether there is any merit in using a polynomial to represent it. Sometimes, of course, it is helpful to use a polynomial as an approximation to another function for which the direct estimation of the parameters would have been difficult or impossible.

VII. FREQUENCY DISTRIBUTIONS

The general topic of frequency distributions is well known to statisticians and fully covered in statistical textbooks. It seems unnecessary, therefore, to include in this paper any lengthy discussion of the subject.

An important class of frequency functions arising from the solutions of a certain first-order differential equation is the Pearsonian system of curves. A comprehensive treatment of this family of curves is given by Elderton[45]. Other good references on the subject, in addition to the writings of Karl Pearson himself, are the discussions given by Peters and Van Voorhis[46], Kenney and Keeping[47], Carver[48], Craig[49], and Kendall[50].

The familiar normal curve is one of the types of curves included in the Pearsonian system. For a discussion of the use of "probability paper" to effect a linear transformation of the integrated normal curve, reference may be made to Finney's Probit Analysis[51].

Methods of parameter estimation commonly used for frequency distributions are the method of moments, the principle of maximum likelihood, and the minimum chi-squared process. These procedures are presented in standard textbooks and in the references given for the Pearsonian curves. It should be noted that the use of these methods is not restricted to the fitting of frequency distributions. An application of the method of maximum likelihood to curve fitting in general as reviewed by Cornell[20], and O'Toole[52] applies the method of moments to a fairly general class of functions.

VIII. SUMMARY

This paper is offered as a guide for those persons who seek to represent experimental data by some appropriate mathematical expression. For straight-line transformations and the general method of differential correction, it should be possible to work directly from this paper. For the other methods treated in less detail, the discussion should serve to indicate the literature available on the particular topic of interest to the experimenter.

It is emphasized that this paper deals with only the various types of curves and the mathematical techniques for fitting them to experimental data. An experimenter needs such general information as a background for the mathematical interpretation of his problem. Another extremely important consideration, however, is the biological or physical significance of the data being analyzed. No mathematical expression can be considered adequate for representing experimental data unless it has evolved from the physical basis of the problem. Such scientific analysis of the problem should be conducted before the techniques of curve fitting are applied.

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