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UCRL LECTURES ON NUMERICAL ANALYSIS AND APPLIED MATHEMATICS

Lecture II

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Berkeley, California

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I. NUMERICAL DIFFERENTIATION

1. Introduction

Formulas for numerical differentiation may be derived in a natural way from the interpolating polynomial formulas. The errors involved may be determined and the methods may then be used to practical advantage.

2. Relations between Differences and Derivatives

By means of induction arguments it may be shown that

$$\text{(a)} \qquad \lim_{\Delta x \to 0} \frac{\Delta^n f(x)}{(\Delta x)^n} = f^{(n)}(x) = \frac{d^n f(x)}{dx^n} \qquad \text{and}$$

$$\text{(b)} \qquad \Delta^n f(x) = (\Delta x)^n f^{(n)}(x + \theta n \Delta x) \text{ where } 0 < \theta < 1 .$$

Relation (b) shows that there is some point between x and $x + n\Delta x$ such that

$$\text{(c)} \qquad f^n(x + n\theta\Delta x) = \frac{\Delta^n f(x)}{(\Delta x)^n} \qquad \text{for } 0 < \theta < 1 .$$

When the function $f(x)$ is unknown, formulas (a) and (c) aid in the evaluation of the error term arising when the difference quotient is

substituted for the derivative.

3. Evaluation of the Error

It may be shown that if $F(x)$ is a polynomial of degree m and is equal to the true function $f(x)$ at $m+1$ points, $x_o, x_1, \ldots, x_m$, then

$$f(x) = F(x) + \frac{(x - x_o)(x - x_1) \ldots (x - x_m)}{(m+1)!} f^{(m+1)}(\xi),$$

where ξ lies in the range x_o to x_m. Differentiating,

$$\frac{df(x)}{dx} = \frac{dF(x)}{dx} + \frac{f^{(m+1)}(\xi)}{(m+1)!} \frac{d}{dx}\left[(x - x_o) \ldots (x - x_m)\right]$$

$$+ \frac{(x - x_o) \ldots (x - x_m)}{(m+1)!} \frac{df^{(m+1)}(\xi)}{dx}.$$

From this equation it may be seen that the error can not be evaluated at every point if $f(x)$ is unknown, since $\frac{df^{(m+1)}(\xi)}{dx}$ can not be evaluated. However, the error can be evaluated at the tabulated points $x_o, x_1, \ldots, x_m$.

Let $g(x) = (x - x_o)(x - x_1) \ldots (x - x_m)$

then

$$\frac{dg(x)}{dx} = \sum_{i=0}^{m} (x - x_o)(x - x_1) \ldots (x - x_{i-1})(x - x_{i+1}) \ldots (x - x_m).$$

$$\left.\frac{dg(x)}{dx}\right|_{x=x_j} = (x_j - x_o)(x_j - x_1) \ldots (x_j - x_{j-1})(x_j - x_{j+1}) \ldots$$

$$\ldots (x_j - x_m).$$

Also $\left.g(x)\right|_{x=x_j} = 0$. Thus the error or remainder term at $x = x_j$ is

$$R(x) = \frac{f^{(m+1)}(\xi)}{(m+1)!}(x_j - x_o)\ldots(x_j - x_{j-1})(x_j - x_{j+1})\ldots(x_j - x_m) .$$

4. Differentiation of Newton's Interpolation Formula.

Newton's interpolation formula in terms of forward differences is

$$F(x) = f(a) + n\Delta f(a) + \frac{n(n-1)}{2!}\Delta^2 f(a) + \ldots + \frac{n(n-1)\ldots(n-m+1)}{m!}\Delta^m f(a)$$

where $x = a + nh$.

Differentiating,

$$F'(x) = \frac{1}{h}\frac{d}{dn}\left[f(a) + n\Delta f(a) + \ldots\right]$$

$$F'(a+nh) = \frac{1}{h}\left[\Delta f(a) + \frac{2n-1}{2}\Delta^2 f(a) + \frac{3n^2 - 6n + 2}{6}\Delta^3 f(a) + \ldots\right]$$

$$F'(a) = \frac{1}{h}\left[\Delta f(a) - \tfrac{1}{2}\Delta^2 f(a) + \tfrac{1}{3}\Delta^3 f(a) + \ldots + \frac{(-1)^{n-1}\Delta^m f(a)}{m}\right] .$$

Evaluating the remainder term for the derivative of Newton's interpolation formula,

$$R = (-1)^m \frac{h^m f^{(m+1)}(\xi)}{m+1} .$$

Now if the analytic form of $f(x)$ is unknown, the best approximation to the error is obtained by approximately evaluating $f^{(m+1)}(\xi)$ by means of relation (c).

$$f^{(m+1)}(\xi) = \frac{\Delta^{m+1} f(x_o)}{(\Delta x)^{m+1}} = \frac{\Delta^{m+1} f(x_o)}{h^{m+1}}$$

since $\xi = x_o + \theta mh$ and $x_o < \xi < x_m$.

Now $R \approx \dfrac{(-1)^m h^m \Delta^{m+1} f(x_o)}{(m+1)\, h^{m+1}} = \dfrac{(-1)^m \Delta^{m+1} f(x_o)}{(m+1)\, h}$.

Thus as h becomes smaller, the approximation becomes better by formula (a).

The second and higher derivatives are obtained the same manner. For example,

$$F''(x) = \frac{1}{h}\frac{d}{dn} F'(a+nh) .$$

5. Comparison of Standard Formulas.

Letting $x = a_o + nh$, the first three terms of the standard formulas are

(a) Newton's

$$F'(a_o + nh) = \frac{1}{h}\left[\Delta f(a_o) + \frac{2n-1}{2}\Delta^2 f(a_o) + \frac{3n^2 - 6n + 2}{6}\Delta^3 f(a_o) + \ldots\right]$$

(b) Stirling's

$$F'(a_o + nh) = \frac{1}{h}\left[\frac{\Delta f(a_{-1}) + \Delta f(a_o)}{2} + n\Delta^2 f(a_{-1}) + \frac{3n^2 - 1}{3!}\,\frac{\Delta^3 f(a_{-2}) + \Delta^3 f(a_{-1})}{2} + \ldots\right]$$

(c) Bessel's

$$F'(a_o + nh) = \frac{1}{h}\left[\Delta f(a_o) + \frac{n}{2}\,\frac{\Delta^2 f(a_{-1}) - \Delta^2 f(a_o)}{2} + \frac{3n^2 - \frac{1}{4}}{3!}\Delta^3 f(a_{-1}) + \ldots\right]$$

Newton's formula is a polynomial of order n and is generally used at the beginning or end of tables. Stirling's formula is a polynomial of

order $2n$ and is used most effectively close to tabulated values, for $|n| < 1/4$, while Bessel's formula of order $2n+1$ is used between $1/4 < n < 3/4$.

For the tabulated values, $n = 0$, the formulas are

<u>Newton's</u> $$F'(a_o) = \frac{1}{h}\left[\Delta f(a_o) - \tfrac{1}{2}\Delta^2 f(a_o) + \tfrac{1}{3}\Delta^3 f(a_o) + \dots\right].$$

<u>Stirling's</u> $$F'(a_o) = \frac{1}{h}\left[\frac{\Delta f(a_{-1}) + \Delta f(a_o)}{2} - \frac{1}{3!}\,\frac{\Delta^3 f(a_{-2}) + \Delta^3 f(a_{-1})}{2} + \dots\right].$$

<u>Bessel's</u> $$F'(a_o) = \frac{1}{h}\left[\Delta f(a_o) - \frac{1}{4\times 3!}\Delta^3 f(a_{-1}) + \dots\right].$$

By observation it is seen that Newton's formula for tabulated values is the easiest to compute with. However, if only first approximations are wanted, then the first term of Stirling's equation is the most satisfactory.

6. Maxima and Minima

These formulas can be used to calculate the value of x at a maximum or minimum. Using Newton's formula, where $x = a_o + nh$,

$$F'(a_o + nh) = 0 = \frac{1}{h}\left[\Delta f(a_o) + \frac{2n-1}{2}\Delta^2 f(a_o) + \frac{3n^2 - 6n + 2}{6}\Delta^3 f(a_o) + \dots\right].$$

Using the first three terms,

$$0 = \tfrac{1}{2} n^2 \Delta^3 f(a_o) + n(\Delta^2 f(a_o) - \Delta^3 f(a) + \left[\Delta f(a) - \tfrac{1}{2}\Delta^2 f(a) + \tfrac{1}{3}\Delta^3 (a)\right].$$

If, upon solving this formula, n is greater than one, then shifting position in the table will improve the solution. Also, taking more terms will improve the accuracy of x.

7. Partial Derivatives

Using the double interpolation formula, $\frac{\partial z}{\partial x}$ and $\frac{\partial z}{\partial y}$ may be computed for $z = f(x, y)$. Using arguments, $x = a_o + uh$ and $y = b_o + vk$, where

$$h = a_1 - a_o = a_2 - a_1 = \cdots = a_m - a_{m-1} \quad \text{and}$$

$$k = b_1 - b_o = b_2 - b_1 = \cdots = b_m - b_{m-1} ,$$

$$z = f(x, y) = z_{oo} + u\Delta^{1+o} z_{oo} + v\Delta^{o+1} z_{oo}$$

$$+ \tfrac{1}{2}\left[u(u-1)\Delta^{2+o} z_{oo} + 2uv\Delta^{1+1} z_{oo} + v(v-1)\Delta^{o+2} z_{oo}\right]$$

$$+ \frac{1}{3!}\left[u(u-1)(u-2)\Delta^{3+o} z_{oo} + 3u(u-1)v\Delta^{2+1} z_{oo} + 3uv(v-1)\Delta^{1+2} z_{oo} + v(v-1)(v-2)\Delta^{o+3} z_{oo}\right] + \cdots$$

where

$$\Delta^{m+n} z_{oo} = \Delta^{m+o} z_{on} - n\Delta^{m+o} z_{o,n-1} + \frac{n(n-1)}{2}\Delta^{m+o} z_{o,n-2} + \cdots + \Delta^{m+o} z_{oo} .$$

or

$$\Delta^{m+n} z_{oo} = \Delta^{o+n} z_{mo} - m\Delta^{o+n} z_{m-1,o} + \frac{m(m-1)}{2}\Delta^{o+n} z_{m-2,o} + \cdots + \Delta^{o+n} z_{oo} ,$$

and $z_{ik} = a_i b_k$.

The error term is derived in Scarborough, first edition.

Differentiating,

$$\frac{\partial z}{\partial x} = \frac{\partial u}{\partial x}\frac{\partial z}{\partial u} = \frac{1}{h}\frac{\partial z}{\partial u}$$

$$\frac{\partial z}{\partial y} = \frac{1}{k}\frac{\partial z}{\partial v}$$

$$\frac{\partial z}{\partial x} = \frac{1}{h}\left\{\Delta^{1+o} z_{oo} + \frac{1}{2!}\left[(2u-1)\Delta^{2+o} z_{oo} + 2v\Delta^{1+1} z_{oo}\right]\right.$$

$$+\frac{1}{3!}\left[(3u^2 - 6u + 2)\Delta^{3+o} z_{oo} + (6u-3)v\Delta^{2+1} z_{oo}\right.$$

$$\left.+3v(v-1)\Delta^{1+2} z_{oo}\right] + \ldots$$

$\frac{\partial z}{\partial y}$ is similarly obtained.

II. CURVE FITTING

1. Introduction

The subject of curve fitting is twofold. First a function must be found to fit the given data and secondly the constants of the function must be evaluated in order to obtain the best fit of the function. The first problem is concerned with finding an empirical function of which there may be many. In the second case the exact functional form of the curve may be known and the problem is to find the best fit to the observational data. Since there is such a large number of possible approximating functions, no systematic method of finding the best empirical function is possible.

2. Graphical Methods

It is very often possible to use function scales which are so chosen that the graph of the function becomes approximately a straight line. Semi-log and log-log graph papers are commonly used.

If $y = k\,a^{mx}$, then $\log y = \log k + (m \log a)x$ and $\log y$ and x are linearly related.

If $y = b\,x^n$ then $\log y = \log b + n \log x$ and $\log y$ and $\log x$ are linearly related.

In general, if $N(y) = m\,\xi(x) + b$, where ξ and N are function scales for x and y, then $\xi(x)$ and $N(y)$ are linearly related.

3. Use of Differences

Using the observed pairs, $(x_i\ y_i)$, a table of differences of the y_i is set up. If the x_i form an arithmetic progression, $x_i - x_{i+1} = k$ for all i, and if the r'th difference of the y_i is constant, all higher

differences being zero, then y is a polynomial in x of degree r. If the r'th difference is almost constant, then a polynomial of degree r will be a good approximation to $y(x)$.

Modifying the conditions on the x's and y's, other possible representations of $y(x)$ may be found. If the values of x_i^n form an arithmetic progression and if the r'th difference of y_i^m is constant or almost constant, then $y_i^m = a_o + a_1 x^n + a_2 (x^n)^2 + \ldots + a_r (x^n)^r$.

If $m = n = -1$ and $r = 1$, then $y = \dfrac{x}{a_1 + a_o x}$ and the function y has asymptotes $x = -\dfrac{a_1}{a_o}$ and $y = \dfrac{1}{a_o}$. In this case $1/y$ versus $1/x$ is a straight line.

If the x_i's form an arithmetic progression and the r'th differences of the y_i form a geometric progression, $\Delta^r y_i = k \Delta^r y_{i+1}$ for all i, then

$$y = a_o + a_1 x + \ldots + a_{r-1} x^{r-1} + k a^x .$$

If $r = 1$, then $y = a_o + k a^x$.

If $a > 1$, then y increases indefinitely with x.

If $0 < a < 1$, then y decreases with x and is asymptotic to $y = a_o$.

Now if the x_i's form a geometric progression, and the y_i's also form a geometric progression, then $y = a x^n$.

4. Evaluation of Arbitrary Constants

4.1 Introduction

Substituting the observational values, (x_i, y_i), $i=1, \ldots, n$, into the approximating function $f(x)$, relationships which the constants must satisfy are obtained.

$$y_i - f(x_i) = 0 \quad \text{for } i = 1, \ldots, n .$$

If there are r, less than n, arbitrary constants, then r of the n equations involving the constants may be selected in hopes of obtaining the best approximation. An alternative is to stipulate that

$$f(x_i) - y_i = f(x_j) - y_j$$

for certain points. However care must be exerted in order that a very large negative error does not cancel a large positive error.

In these two common procedures there is no systematic method, nor is there a reliable estimate of the probable error at every point, nor is there assurance that the best fit has been found. On the other hand the method of least squares has the advantage that it satifies these three requirements.

4.2 Method of Least Squares.

If the function $y(x)$ is to be approximated by

$$f(x) = \sum_{k=o}^{m} a_k \, g_k(x)$$ where the $g_k(x)$ are linearly

independent and $n > m$, then the method of least squares asserts that the residuals $v_i = f(x_i) - y(x_i)$ should be such that $\sum_{i=1}^{n} v_i^{\,2}$ is a minimum.

By partially differentiating $\sum_{i=1}^{n} v_i^2$ with respect to the $m+1$ arbitrary constants and equating to zero, the "normal equations" are obtained which must be satisfied by the arbitrary constants in order that $\sum_{i=1}^{n} v_i^2$ shall be a minimum.

$$a_o \sum_{i=1}^{n} g_o^2(x_i) + a_1 \sum_{i=1}^{n} g_o(x_i)g_1(x_i) + \cdots + a_m \sum_{i=1}^{n} g_o(x_i)g_m(x_i)$$

$$= \sum_{i=1}^{n} g_o(x_i)y(x_i) \quad .$$

$$a_o \sum_{i=1}^{n} g_1(x_i)g_o(x_i) + a_1 \sum_{i=1}^{n} g_1^2(x_i) + \cdots + a_m \sum_{i=1}^{n} g_1(x_i)g_m(x_i)$$

$$= \sum_{i=1}^{n} g_1(x_i)y(x_i) \quad .$$

....

....

$$a_o \sum_{i=1}^{n} g_m(x_i)g_o(x_i) + a_1 \sum_{i=1}^{n} g_m(x_i)g_1(x_i) + \cdots + a_m \sum_{i=1}^{n} g_m^2(x_i)$$

$$= \sum_{i=1}^{n} g_m(x_i)y(x_i) \quad .$$

There are $m+1$ equations in the $m+1$ unknowns, $a_o, a_1, \ldots, a_m$. There will be a solution if the determinant of the coefficients is not zero.

4.3 Applications of Least Square Method

4.31 Linear Functions

If y is to be approximated by $f(x) = ax + b$, then the normal equations are

$$bn + a \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$

$$b \sum_{i=1}^{n} x_i + a \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i$$

or

$$a = \frac{\sum x_i \sum y_i - n \sum x_i y_i}{\sum x_i \sum x_i - n \sum x_i^2}$$

and

$$b = \frac{\sum x_i y_i \sum x_i - \sum y_i \sum x_i^2}{\sum x_i \sum x_i - n \sum x_i^2}$$

4.32 Polynomials

Let $f(x) = a_o + a_1 x + a_2 x^2 + \ldots + a_n x^n$.

In order to simplify the problem, x will be transformed so that the interval (a, b) in which we are interested becomes the interval $(-1, +1)$.

Then $x = \frac{a+b}{2} - \frac{a-b}{2} t$ and $f(t) = c_o + c_1 t + c_2 t^2 + \ldots + c_n t^n$ where $g_k(t) = t^k$. Now $\sum_{i=1}^{n} t_i^{2k+1} = 0$ when y is tabulated in equal intervals of x. The normal equations become

$$nc_o + c_2 \sum t_o^2 + c_4 \sum t_i^4 + \ldots = \sum y_i$$

$$c_1 \sum t_i^2 + c_3 \sum t_i^4 + \ldots = \sum t_i y_i$$

$$c_o \sum t_i^2 + c_2 \sum t_i^4 + c_4 \sum t_i^6 + \ldots = \sum t_i^2 y_i$$

....

The normal equations thus divide into two groups, one with even numbered coefficients and the other with odd numbered coefficients. The solution now is much easier to find.

4.33 Computing procedures

The following examples are given to illustrate how the work of computation with a calculator may be reduced. A tabulation form with positive checks is illustrated since most mistakes enter into the calculations at the stage of tabulation. The abridged form for solving the normal equations is simple but the computer must be careful of the loss of significant figures since the process may involve subtraction of numbers of the same order of magnitude.

Example 1: Applied least square method.

Let $z(x\ y) = a\,x + b\,y + c$ where (x_i, y_i, z_i) are observed values.

$$\sum_{i=1}^{n} v_i^2 = \sum_{i=1}^{n} (a\,x_i + b\,y_i + c - z_i)^2$$

$$\frac{\partial \sum v_i^2}{\partial a} = 0 \;; \quad \frac{\partial \sum v_i^2}{\partial b} = 0 \;; \quad \frac{\partial \sum v_i^2}{\partial c} = 0 \;.$$

$$nc + a\sum x_i + b\sum y_i = \sum z_i$$

$$c\sum x_i + a\sum x_i^2 + b\sum x_i\,y_i = \sum x_i\,z_i$$

$$c\sum y_i + a\sum y_i\,x_i + b\sum y_i^2 = \sum y_i\,z_i \;.$$

Tabulation with positive checks

x_i	y_i	z_i	x_i^2	$x_i y_i$	y_i^2	$x_i z_i$	$y_i z_i$
x_1	y_1	z_1					
x_2	y_2	z_2					
x_3	y_2	z_3	accumulate these on machine				
$\vdots$	$\vdots$	$\vdots$					
x_n	y_n	z_n					
$\sum x_i$	$\sum y_i$	$\sum z_i$	$\sum x_i^2$	$\sum x_i y_i$	$\sum y_i^2$	$\sum x_i z_i$	$\sum y_i z_i$

$1 + x_i + y_i$	$(1 + x_i + y_i)^2$	$z_i(1 + x_i + y_i)$
$1 + x_1 + y_2$		
$1 + x_2 + y_2$		
$1 + x_3 + y_3$	accumulate on machine	
$\vdots$	$\vdots$	$\vdots$
$1 + x_n + y_n$		
$\sum (1 + x_i + y_i)$	$\sum (1 + x_i + y_i)^2$	$\sum z_i(1 + x_i + y_i)$

Checks:

1. $$\sum (1 + x_i + y_i) = \sum x_i + \sum y_i + n$$

2. $$\sum (1 + x_i + y_i)^2 = \sum x_i^2 + \sum y_i^2 + 2\sum x_i y_i + \sum x_i + \sum y_i + n$$

3. $$\sum z_i(1 + x_i + y_i) = \sum z_i + \sum z_i x_i + \sum z_i y_i .$$

Example 2: Doolittle's Abridged Method.

Let the normal equations be

$$a_{oo}\, k + a_{1o}\, \ell + a_{2o}\, m = b_o$$

$$a_{o1}\, k + a_{11}\, \ell + a_{21}\, m = b_1$$

$$a_{o2}\, k + a_{12}\, \ell + a_{22}\, m = b_2 \qquad \text{where } a_{k\ell} = a_{\ell k} .$$

					check column
I.	a_{oo}	a_{1o}	a_{2o}	b_o	$b_o + a_{oo} + a_{1o} + a_{2o}$
(2)		a_{11}	a_{21}	b_1	$b_1 + a_{1o} + a_{11} + a_{21}$
(3)			a_{22}	b_2	$b_2 + a_{2o} + a_{21} + a_{22}$
(2)		a_{11}	a_{21}	b_1	$b_1 + a_{1o} + a_{11} + a_{21}$
(4)	$I \times \frac{-a_{1o}}{a_{oo}}$	$\frac{-a_{1o}a_{1o}}{a_{oo}}$	$\frac{-a_{2o}a_{1o}}{a_{oo}}$	$\frac{-b_o a_{1o}}{a_{oo}}$	$\frac{-a_{1o}}{a_{oo}}\left[b_o + a_{oo} + a_{1o} + a_{2o}\right]$

II.	(2) + (4)	a'_{11}	a'_{21}	b'_1	$b'_1 + a'_{11} + a'_{21}$ (check)
	(3)		a_{22}	b_2	$b_2 + a_{20} + a_{21} + a_{22}$
	(5) I x $\frac{-a_{20}}{a_{00}}$		$a_{20}\frac{-a_{20}}{a_{00}}$	$b_0\frac{-a_{20}}{a_{00}}$	$\frac{-a_{20}}{a_{200}}\left[b_0 + a_{00} + a_{10} + a_{20}\right]$
	(6) II x $\frac{-a'_{21}}{a'_{11}}$		$a'_{21}\frac{a'_{21}}{a'_{11}}$	$b_2\frac{-a'_{21}}{a'_{11}}$	$\frac{-a'_{21}}{a'_{11}}\left[b'_1 + a'_{11} + a'_{21}\right]$
III.	(3) + (5) + (6)		a'_{22}	b'_2	b'_2 a'_{22} (check)

Now the normal equations can be solved easily.

$$a'_{22}\, m = b'_2$$

$$a'_{11}\,\ell + a'_{21}\, m = b'_1$$

$$a_{00}\, k + a_{10}\,\ell + a_{20}\, m = b_0 .$$

4.4 Integral Cases

If continuous curves rather than discrete observations are being considered, then $\int_a^b \left[f(x) - y(x) \right]^2 dx$ is minimized. In the normal equations $\int_a^b$ is substituted for $\sum_{i=1}^{n}$. Transforming the interval

(a, b) to (-1, +1), there are terms like $\int_{-1}^{+1} g_m(t) g_n(t)\, dt$ where

$$f(t) = \sum_{m=0}^{n} a_m t^m \quad \text{and} \quad g_m(x) = x^m$$

and $g_m(t) = t^m$.

For the general term,

$$\int_{-1}^{+1} g_m(t)\, g_\ell(t) dt = \int_{-1}^{+1} g^{m+\ell}\, dt = \begin{cases} \dfrac{2}{m+\ell+1} & m+n \text{ odd} \\ 0 & m+n \text{ even} \end{cases}$$

The other terms are

$$\int_{-1}^{+1} g_k(t)\, y\, dt = \int_{-1}^{+1} t^k\, y\, dt$$

$$2\, J_o = \int_{-1}^{+1} y\, dt$$

$$2\, J_1 = \int_{-1}^{+1} y\, t\, dt$$

$$2\, J_2 = \int_{-1}^{+1} y\, t^2\, dt, \quad \text{etc.}$$

The normal equations are now

$$a_o + \frac{1}{3} a_2 + \frac{1}{5} a_4 + \ldots = J_o$$

$$\frac{1}{3} a_1 + \frac{1}{5} a_3 + \frac{1}{7} a_5 \ldots = J_1$$

$$\frac{1}{3} a_o + \frac{1}{5} a_2 + \frac{1}{7} a_4 + \ldots = J_2$$

etc.

This set of normal equations divides into odd and even groups and the a's can be written in terms of the J's.

The disadvantage of the power series approximation is that the constants must be reevaluated if additional terms are added for greater accuracy.

If orthogonal polynomials are used, then only the diagonal terms in the normal equations remain and, as a consequence, the previous calculations do not change with the addition of more terms. Then

$$a_k = \frac{1}{b_k} \int_{-1}^{+1} g_k(t)\, y\, dt \qquad \text{where}$$

$$b_k = \int_{-1}^{+1} \left[g_k(t) \right]^2 dt .$$

4.5 Fundamental Theorem.

The fundamental theorem states that the approximating function determined by the least square method is closer to the true function than the observed function.

Let z be a continuous function in (a, b) which is to be approximated by

$$y(x) = \sum_{i=1}^{m} a_i v_i(x) \quad \text{where}$$

$v_1(x), v_2(x), \ldots, v_m(x)$ are linearly independent continuous functions of x in the interval (a, b). The a's are determined so as to minimize the integral

$$I = \int_a^b w(z - \sum_{i=1}^{m} a_i v_i)^2 \, dx \qquad \text{where} \quad w(x), \text{ a weight}$$

function, is a continuous non-negative function of x in (a, b).

Now $z(x)$ has been obtained from observations subject to random errors. There is a true function $u(x)$ which would have been found if there were no errors in observation.

<u>Theorem:</u> If the true function $u(x)$ can be represented by v's, which are linearly independent, so that

$$u(x) = b_1 v_1 + b_2 v_2 + \ldots \quad b_n v_n \; ,$$

and if a's are determined so that

$$y(x) = a_1 v_1 + a_2 v_2 + \ldots + a_n v_n$$

is the least square approximation to the observed function $z(x)$, then

$$\int_a^b w(z - u)^2 \, dx = \int_a^b w(z - y)^2 \, dx + \int_a^b w(y - u)^2 \, dx \quad .$$

This states that except for $y \equiv z$, a trivial case,

$$\int_a^b w(y - u)^2 \, dx < \int_a^b (z - u)^2 \, dx$$

or that y is closer to the true function than z, the observed function.

4.6 Non-linear Cases

It was previously assumed that the arbitrary constants appeared linearly in the equations. This is not the case in general. Consequently if this method is to be applied to non-linear equations, they must be transformed by some means into a linear form.

If $N(y) = a\,\xi(x) + b$ and if (x_i, y_i) are the observational values, then

$$\Delta N_i = N_i - a\,\xi_i - b \approx N'(y_i)\,\Delta y_i$$

$$\Delta y_i = \frac{\Delta N_i}{N'(y_i)} = \frac{N_i}{N'(y_i)} - a\,\frac{\xi_i}{N'(y_i)} - b\,\frac{1}{N'(y_i)} .$$

The normal equations are

$$\frac{\partial \sum \Delta y_i^2}{\partial b} = 0 = \sum \frac{N_i}{\left[N'(y_i)\right]^2} - a \sum \frac{\xi_i}{\left[N'(y_i)\right]^2} - b \sum \frac{1}{\left[N'(y_i)\right]^2}$$

$$\frac{\partial \sum \Delta y_i^2}{\partial a} = 0 = \sum \frac{N_i\,\xi_i}{\left[N'(y_i)\right]^2} - a \sum \frac{\xi_i^2}{\left[N'(y_i)\right]^2} - b \sum \frac{\xi_i}{\left[N'(y_i)\right]^2}$$

If it is not possible to transform the equations into a linear form, but if an approximate solution to the problem is known, then by means of a Taylor's expansion about the approximate solution, a linear equation for correction terms can be written. This is sometimes called a differential correction method.

Let $y = f(x, a, b, c)$ be the equation involving the constants in a non-linear way and let a_o, b_o, c_o be a known approximate solution. We wish

$$a = a_o + \Delta a$$
$$b = b_o + \Delta b$$
$$c = c_o + \Delta c \quad \text{where } \Delta a, \Delta b, \Delta c \text{ are small.}$$

$$v_i = f(x_i, a, b, c) - y_i$$

$$v_i = \left[f(x_i, a_o + \Delta a, b_o + \Delta b, c_o + \Delta c) - y_i \right]$$

$$= \left[f(x_i, a_o, b_o, c_o) + \frac{\partial f}{\partial a}(x_i, a_o, b_o, c_o)\Delta a \right.$$

$$+ \frac{\partial f}{\partial b}(x_i, a_o, b_o, c_o)\Delta b + \frac{\partial f(x_i, a_o, b_o, c_o)}{\partial c}\Delta c$$

$$\left. + \text{higher order terms} \right] - y_i$$

If the higher order terms are neglected, then Δa, Δb, Δc will be in a linear form and the terms for the normal equations can be computed. This gives a solution for Δa, Δb, Δc. Repetition of this process will provide a check on the omputation and will also improve the evaluation of a, b, and c to within the limits of the experimental error.

5. Criticism

It must be recognized that the argument was assumed all along to be exact. This is not true in general for most experimental data. It is hoped that the error made in assuming the argument exact is small and unimportant in the desired answer.

If the error in the argument is of the same order of magnitude as that in the function, then two curves could be drawn through a given set of points, one for exact argument and one for exact function.

It is presumed that the best curve lies between these curves. However the real advantage of the least square fit is now lost since there is no way of judging the best fit or the error involved.

The best discussion of the estimation of errors is found in Birge's notes.

6. Bibliography

6.1 Milne, "Numerical Calculus".

6.2 Sokolinkoff, "Higher Mathematics for Engineers and Physicists".

6.3 Willer, "Practical Analysis".

6.4 Scarborough, "Numerical Mathematical Analysis".

6.5 Birge, R. T., Chairman of Physics Department, University of California, Lecture notes for Physics 204.