ISSN-0976-2124

Volume 3	Number 2	December 2010

Hislopia Journal

A National Journal of

* Science and Technology
* Arts and Humanities
* Commerce and Management
* Human development

Published by
Hislop College, Civil Lines, Nagpur- 440 001 (MS) India

The 'Hislopia Journal' (ISSN 0976-2124) is a biannual (June and December), peer reviewed journal publishing original research papers, short communications and reviews on all aspects of Science, Humanities, Arts, Linguistics, Commerce and Management. The journal is named after Rev. Stephen Hislop, the founder of Hislop College, Nagpur who was not only an Evangelist and Educationist, but also a renowned scientist and researcher in the field of Geology and Linguistics. This journal will cater to the research aptitude of college teachers, researchers and scientists of Central India, in particular and the country in general.

Annual Subscription Information

Individual.............	Rs. 500/-	(Inland)
	US$ 50/-	(Overseas)
Institutional...........	Rs. 1000/-	(Inland)
	US$ 100/-	(Overseas)

Payment towards annual subscription should be made by a Bank Demand Draft in favour of 'Hislop Education Society' payable at Nagpur.

Hislopia Journal 3 (2) 2010 209-219
ISSN-0976-2124

CURVE FITTING, INTERPOLATION & EXTRAPOLATION

AN INTERACTIVE APPROACH

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Abstract **Experimental data are often seen graphically by analytical minds. Then the desires for its fitting into curve and line is obvious for learning its trend and analysis. Interpolations and permitted extrapolations are also required for various purposes that include calibrations and extreme analysis**

Keywords **interactive capabilities, graphical output, interpolations, extrapolations, quasi-continuous, least square, best fit, caliberation**

Introduction

Numerical problems in theoretical physics was the domain of large computers, until a few years ago. Now-a-days, personal computers have reached the power at par with large computers of early sixties. Apart from their high computational performances, personal computers offer interactive capabilities and rapid graphical output of results. Thus, the personal computers offer us a wide field of possibilities in education and research. The present work is an attempt to fit a continuous experimental data points into the leastsquare equations of five different kinds.

(1) Equation of a Line:

$y = mx + c$

(2) Exponential Function:

$y = aebx$

(3)Logarithmic Function:

$y = a \ln (x) + b$

(4) Power Function:

$y = axb$

(5) Polynomial Function (Order 3):

$y = f x = a + a x + a x + a x$

These equations are then capable of generating interpolations and extrapolations between

and beyond data points (if feasible). The perfect-ness of the equation with data can be judged from deviations e.g. the equation (out of five) for which standard deviation (SD) is minimum is closest to the data and is the best-fit-equation. Visualizing a graph from data points and generated equation with quasi-continuous interpolated data gives an exciting glimpse. The C++ programme sample example depicted in the Appendix will help the users to take a ride on their PC with their experimental data and an equation.

Theory of Approximation by Least-Squares

1. Discrete data and equation of least-square line

The general equation of a straight line with slope m and y-intercept c is:

$y = mx + c$ (1)

The Least-Square Principle (Linear)

The basic idea of choosing a linear approximation $p(x)$ to give function $y(x)$ in a way which minimizes the square of the errors (in some sense), was developed first by Gauss.

There are several variations, depending upon the set of arguments involved and the error measure to be used.

First of all, *when the data are discrete* we may minimize the sum

$$s = \sum_{0}^{N}[y_i - mx_i - c]^2$$

for given data (xi, yi) and parameters to be found are m and c. The mathematical condition for solving set equations (2) for m and c is that the set of equations should be two or more. That is, the data points for which we are finding equation of a straight line should be at least two ore more. In equation (2) S probably cannot be made zero. The idea of Gauss is to make S as small as we can. Mathematically, at $= \frac{\partial S}{\partial m} = 0, \frac{\partial S}{\partial c} = 0$ the square function S will have minima . The standard techniques of calculus then lead to *the normal equations*, which determine the coefficients. These equations are

$$ms_2 - cs_1 = t_1$$
$$ms_1 - cs_0 = t_0 \quad .(3)$$

where $S_k = \sum_{i=0}^{N} x_i^k, t_k = \sum_{i=0}^{N} y_i x_i^k$

.This system of linear equations does determine the m and c uniquely, and the resulting coefficients do actually produce the minimum possible value of S. For the case of linear polynomial

$p(x) = c + mx$

The normal equations are easily solved and yield slope and y-intercept

$$m = \frac{s_0 t_1 - s_1 t_0}{s_0 s_2 - s^2_1} \quad c = \frac{s_2 t_0 - s_1 t_1}{s_0 s_2 - s^2_1} \quad ....(4)$$

2. Discrete data and exponential function

The general exponential equation for relating x and y be:

$$y_i = ae^{bx_1} \quad ... \quad (5)$$

The Least-Square Principle (Exponential)

$\log y_i = \log a + bx_i$

First of all, *when the data are discrete* we may minimize the sum

$$S = \sum_{i=0}^{N}[\log y_i - \log a - bx_i]^2 \quad ...(6)$$

for given data (xi, yi) and parameters to be found are a and b. The mathematical condition for solving set equations (6) for a and b is that the set of equations should be two or more.

In equation (6) S probably cannot be made zero. The idea of Gauss is to make S as small as we can. Mathematically, at $\frac{\partial s}{\partial a}=0, \frac{\partial s}{\partial b}=0$ the square function S will have minima .

The standard techniques of calculus then lead to *the normal equations,* which determine the coefficients. These equations are

$$\log as_0 + bs_1 = t_o$$
$$\log as_1 + bs_2 = t_1 \quad \text{..... (7)}$$

where $\sum_{i=0}^{N} .x_i^k, t_k = \sum_{i=0}^{N} \log(y_i) x_i^k$

This system of linear equations does determine the a and b uniquely, and the resulting coefficients do actually produce the minimum possible value of S.

The normal equations are easily solved and yield slope and y-intercept

$$b = \frac{s_o t_1 - s_1 t_0}{s_o s_2 - s^2{}_1}, a = \exp\left(\frac{s_2 t_0 - s_1 t_1}{s_o s_2 - s^2{}_1}\right) 8$$

3. Discrete data and logarithmic function

The general exponential equation for relating x and y be:

$$y = a \log x + b \quad (9)$$

The Least-Square Principle (Logarithmic)

$$y_i = a \log b_i + x$$

First of all, *when the data are discrete* we may minimize the sum

$$S = \sum_{i=0}^{N} [y_i - a \log x_i - b]^2 \quad \text{....(10)}$$

for given data (x_i, y_i) and parameters to be found are a and b. The mathematical condition for solving set equations (10) for a and b is that the set of equations should be two or more. In equation (10) S probably cannot be made zero. The idea of Gauss is to make S as small as we can.

Mathematically, at $\frac{\partial s}{\partial a}=0, \frac{\partial s}{\partial b}=0$ the square function S will have minima . The standard techniques of calculus then lead to *the normal equations*, which determine the coefficients. These equations are

$$bs_o + as_1 = t_0$$
$$bs_1 + as_2 = t_1 \quad \text{..... .(11)}$$

where

$$S = \sum_{i=0}^{N} (\log x_i)^k, t_k = \sum_{i=0}^{N} y_i (\log x_i)^k$$

This system of linear equations does determine the a and b uniquely, and the resulting coefficients do actually produce the minimum possible value of S.

The normal equations are easily solved and yield slope and y-intercept

$$a = \frac{s_o t_1 - s_1 t_0}{s_o s_2 - s^2{}_1}, b = \frac{s_2 t_0 - s_1 t_1}{s_o s_2 - s^2{}_1} \quad \text{....(12)}$$

4. Discrete data and Power function

The general power equation for relating x and y be:

$$y = ax_b \quad \text{... (13)}$$

The Least-Square Principle (Logarithmic)

$y_i = \log a + b\log x_i$

First of all, *when the data are discrete* we may minimize the sum

$$S = \sum_{i=0}^{N}[y_i - \log a + b\log x_i]^2, t_k \quad (14)$$

for given data (x_i, y_i) and parameters to be found are a and b. The mathematical condition for solving set equations (14) for a and b is that the set of equations should be two or more. In equation (14) S probably cannot be made zero. The idea of Gauss is to make S as small as we can.

Mathematically, at $\frac{\partial s}{\partial a} = 0, \frac{\partial s}{\partial b} = 0$ the square function S will have minima . The standard techniques of calculus then lead to *the normal equations*, which determine the coefficients. These equations are

$$\log a s_0 \; b s_1 = t_0$$
$$\log a s_1 \; b s_2 = t_1 \quad (15)$$

where s_k

$$S = \sum_{i=0}^{N}(\log x_i)^k, t_k = \sum_{i=0}^{N}\log y_i \times (\log x_i)^k$$

This system of linear equations does determine the a and b uniquely, and the resulting coefficients do actually produce the minimum possible value of S.

The normal equations are easily solved and yield slope and y-intercept

$$b = \frac{s_o t_1 - s_1 t_0}{s_o s_2 - s^2_1}, a = \exp\left(\frac{s_2 t_0 - s_1 t_1}{s_o s_2 - s^2_1}\right) \quad ....(16)$$

5. Discrete data and Least-Square Polynomial (Non-linear)

An expression to a general polynomial of order m (our case is m=3) is

$$y = f(x) = a_0 + a_1 x - a_2 x^2 + ... + a_m x^m$$

$$= \sum_{i=0}^{m} a_i x^i \quad ....(17)$$

In generalizing the problem of linear polynomial, setting derivatives of S relative to $a_0, a_1, a_2, a_3 .... a_m$ to zero produces $m+1$ equations for polynomial

$$\frac{\partial S}{\partial a_k} = -2\sum_{i=0}^{N} x_i^k [y_i - a_0 - a_1 x_i - a_2 x_i^2$$

$$- .. - a_m x_i^m] = 0 ...(18)$$

where $k = 0,...,m$. Introducing symbols

$S_k = \sum_{i=0}^{N} x_i^k, t_k = \sum_{i=0}^{N} y_i x_i^k$ these equations may be re-written as (18) and are called as *normal equations.*

$$s_0 a_0 + s_1 a_1 + ... + s_m a_m = t_0$$
$$s_1 a_0 + s_2 a_1 + ... + s_{m+1} a_m = t_1$$
$$\text{---------------------------------} \quad ...(19)$$
$$s_m a_0 + s_{m+1} a_1 + ... + s_{2m} a_m = t_m$$

Solving for the coefficients ai we obtain the least square polynomial. There is a unique solution and that it minimize S. For small integers m, may be solved without difficulty.

However for large m the system is badly ill-conditioned. Solution to such system does exist but is beyond the scope now. Therefore, while accepting the data it has been asked in the programme that user should provide at-least four data points as we are evaluating four coefficients a_0, a_1, a_2, a_3 to part from mathematical ill-condition.

Note: the number of data points N used for least-square processing and degree of polynomial m desired should always maintain relation $N > m$.

Simultaneous Linear Equations

Simultaneous $m+1$ linear equations (19) raise in m unknowns can be solved by Cramer's delta rule.

If the $(m \times m)$ determinant

$$\Delta = \begin{vmatrix} S_0 & S_1 & S_2 & \cdots & S_m \\ S_1 & S_2 & S_3 & \cdots & S_{m+1} \\ S_2 & S_3 & S_4 & \cdots & S_{m+2} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ S_m & S_{m+1} & S_{m+2} & \cdots & S_{2m} \end{vmatrix} \quad (20)$$

is not zero, then solutions of equations (3) is given by Cramer's rule as

$$a_o = \frac{D_1}{\Delta}, a_1 = \frac{D_2}{\Delta}, a_2 = \frac{D_3}{\Delta}, \ldots, = \frac{D_{m+1}}{\Delta}$$

where the $(m \times m)$ determinant,

$$D_l = \begin{vmatrix} S_0 & S_1 & \cdots & S_{l-1} & t_0 & S_{l+1} & \cdots & S_m \\ S_1 & S_2 & \cdots & S_l & t_1 & S_{l+2} & \cdots & S_{m+1} \\ S_2 & S_3 & \cdots & S_{l+1} & t_2 & S_{l+3} & \cdots & S_{m+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ S_m & S_{m+1} & \cdots & S_{l+m} & t_m & S_{l+l+m} & \cdots & S_{2m} \end{vmatrix} \quad \ldots\ldots.(21)$$

Thus Dl is the same as D except t's replacing s's in the lth column.

Programming in Borland Turbo C++

The programme is devised to accept a number of data points (i) as desired by the user and stored in arrays $x[i]$ and $y[i]$. Using the general polynomial equation of the form

$$y = (f)\, x = a_0 + a_1 x + a_2 x^2 + a_3 x^3$$

we can generate i number of equations out of i data points which are stored in array.

Now these i equations are solved simultaneously for a_0, a_1, a_2, a_3. The following summations are estimated using *for* loop:

$$\sum_1^i x[n], \quad \sum_1^i x^2[n], \quad \sum_1^i x^3[n],$$

$$\sum_1^i x^4[n], \quad \sum_1^i x^5[n], \quad \sum_1^i x^6[n],$$

$$\sum_1^i y[n], \quad \sum_1^i y[n] \times x[n],$$

$$\sum_1^i y[n] \times x[n]^2, \quad \sum_1^i y[n] \times x[n]^3,$$

and assigned with a array $a[p][q]$ and $b[p]$ as:

2 Dimensional

$$a[1][1]=1; \quad a[1][2]=\sum_{1}^{i} x[n]; \quad a[1][3]=\sum_{1}^{i} x^2[n]; \quad a[1][4]=\sum_{1}^{i} x^3[n];$$

$$a[2][1]=\sum_{1}^{i} x[n]; \quad a[2][2]=\sum_{1}^{i} x^2[n];$$

$$a[2][3]=\sum_{1}^{i} x^3[n]; \quad a[2][4]=\sum_{1}^{i} x^4[n];$$

$$a[3][1]=\sum_{1}^{i} x^2[n]; \quad a[3][2]=\sum_{1}^{i} x^4[n];$$

$$a[3][3]=\sum_{1}^{i} x^4[n]; \quad a[3][4]=\sum_{1}^{i} x^4[n];$$

1 Dimensional

$$b[1]=\sum_{1}^{i} y[n], \qquad b[2]=\sum_{1}^{i} y[n]\times x[n];$$

$$b[3]=\sum_{1}^{i} y[n]\times x[n]^2, \; b[4]=\sum_{1}^{i} y[n]\times x[n]^3;$$

Then the following 5 determinants D, D_{oo}, D_{01}, D_{02}, D_{03} are solved for a_0, a_1, a_2, a_3 as:

$$\Delta=\begin{vmatrix} a[1][1] & a[1][2] & a[1][3] & a[1][4] \\ a[2][1] & a[2][2] & a[2][3] & a[2][4] \\ a[3][1] & a[3][2] & a[3][3] & a[3][4] \\ a[4][1] & a[4][2] & a[4][3] & a[4][4] \end{vmatrix},$$

$$\Delta_{oo}=\begin{vmatrix} b[1] & a[1][2] & a[1][3] & a[1][4] \\ b[2] & a[2][2] & a[2][3] & a[2][4] \\ b[3] & a[3][2] & a[3][3] & a[3][4] \\ b[4] & a[4][2] & a[4][3] & a[4][4] \end{vmatrix}$$

$$\Delta = \begin{vmatrix} a[1][1] & b[1] & a[1][3] & a[1][4] \\ a[2][1] & b[2] & a[2][3] & a[2][4] \\ a[3][1] & b[3] & a[3][3] & a[3][4] \\ a[4][1] & b[4] & a[4][3] & a[4][4] \end{vmatrix}$$

$$\Delta_{00} = \begin{vmatrix} a[1][1] & a[1][2] & b[1] & a[1][4] \\ a[2][1] & a[2][2] & b[2] & a[2][4] \\ a[3][1] & a[3][2] & b[3] & a[3][4] \\ a[4][1] & a[4][2] & b[4] & a[4][4] \end{vmatrix}$$

$$\Delta_{03} = \begin{vmatrix} a[1][1] & a[1][2] & a[1][3] & b[1] \\ a[2][1] & a[2][2] & a[2][3] & b[2] \\ a[3][1] & a[3][2] & a[3][3] & b[3] \\ a[4][1] & a[4][2] & a[4][3] & b[4] \end{vmatrix}$$

Using Cramer's rule, the coefficients can be calculated as:

$$a_0 = \frac{\Delta_{a_0}}{\Delta}, a_1 = \frac{\Delta_{a_1}}{\Delta}, a_2 = \frac{\Delta_{a_3}}{\Delta}, a_3 = \frac{\Delta_{a_3}}{\Delta}$$

The case of polynomial is discussed above in detail explains the methodology. For rest of the four equations the summations are to be evaluated as discussed in theory. Rest of the treatment is alike.

(**Note:** Array assignment can be conveniently used for solving 4× 4 determinant and later same solution can be used for replacing columns by *a*[*p*][1]=*b*[*p*], *a*[*p*][2]=*b*[*p*], *a*[*p*][3]=*b*[*p*], *a*[*p*][4]=*b*[*p*] for calculating $\Delta_{\alpha o}, \Delta_{\alpha 1}, \Delta_{\alpha 2}, \Delta_{\alpha 3}$)

Thus, the desired polynomial $y = f(x) = a_o + a_1 x + a_2 x^2 + a_3 x^3$ is known as are known.

Checking the correctness of Best-fit Equations from Deviations

The degree of correctness of predicting a *y* value for any *x* can be systematically understood from deviations

We have already entered points (*xi*,*yi*) in array *x*[*i*], *y*[*i*]. Now, we can calculate array *yc*[*i*] from polynomial and immediately find deviations in array be equation *d*[*i*]=*y*[*i*]-*yc*[*i*].

The **Mean Deviation** $\left(\bar{d}\right)$ can be found by summing all deviations together using a *for* loop and averaging it out as:

$$\bar{d}\frac{1}{n}\sum_{i} d[i] \qquad \text{....(9)}$$

The **Standard Deviation**(σ) can be similarly found by summing all deviation squares together using a *for* loop and averaging it out its root as:

$$\sigma = \sqrt{\frac{1}{n}\sum_{i} d^2[i]}$$

The statements used in programme are depicted in Appendix-I.

Conclusion

Programme devised is empowered to accept any number (32k) of data points for finding Least-Square equation of any type of the prescribed five equations. The generated equation is capable of interpolation and extrapolations which is often required for introspection. The polynomial generated can be the boon for fine calibration when linear fitting affect accuracy due to a small non-linearity in the data. The present programme can interpolate/ extrapolate which can minimize error to a considerable extent and also suggest kind of equation that best-fits data point which is evident from standard deviation. Deviation data displayed at last is indicative of the degree of accuracy claimed for the particular case. The coefficients generated using programme can be used for theoretical interpretation and assimilation of the mechanism of correlation between the parameters on respective axis. Thus, the programme which is a tool for finding Least Square equation is useful for a variety of causes.

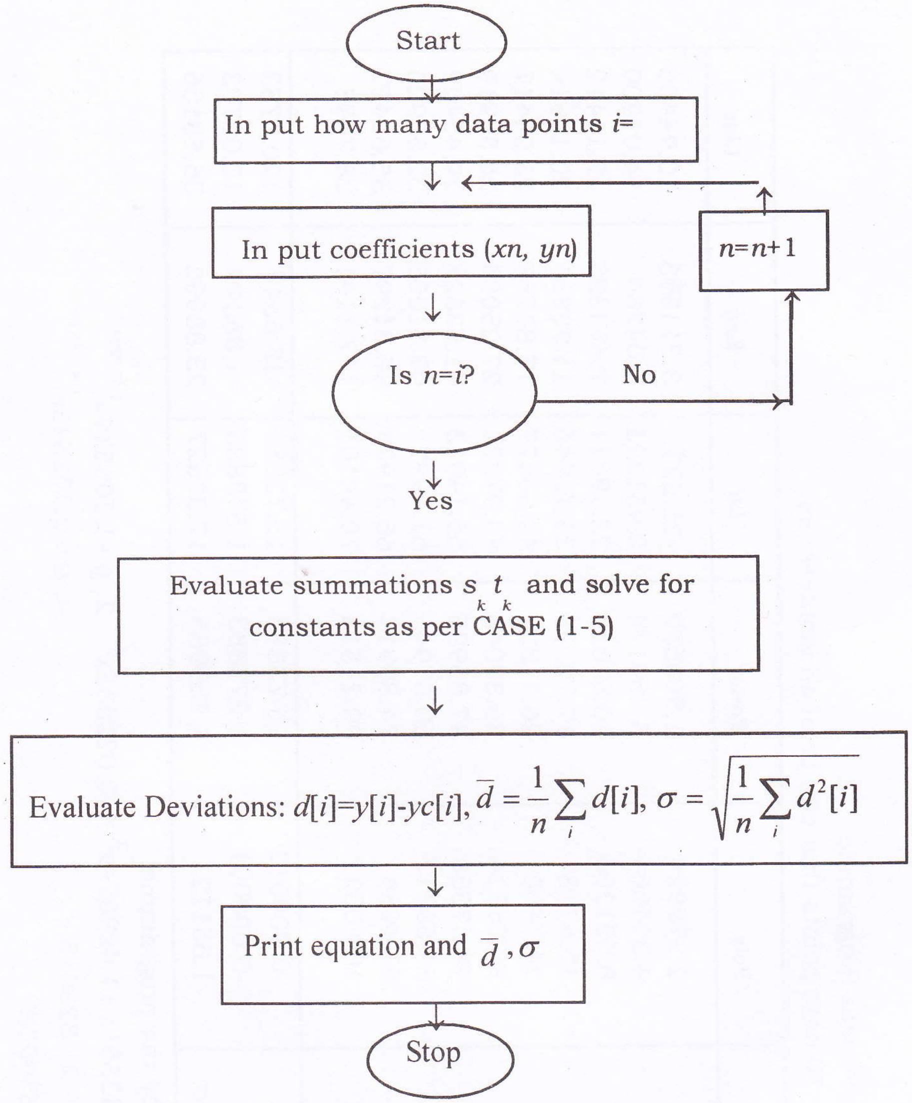

Fig.1: Flow Chart of the Programme

1

Appendix-I

Exercise: Check correctness Programme

Ex 1: We shall enter 10 data points that can be of an isotherm as:

Sr No	x	y	Poly	Power	Ln	Exp	Line
1.	1	2	2.276924	1.506539	-21.823	3.311593	10.94406
2.	2	4	4.204664	5.164172	5.951223	5.04784	14.02909
3.	3	10	8.681356	10.61616	22.19811	7.694389	17.11412
4.	4	15	15.5718	17.70195	33.72546	11.72851	20.19914
5.	5	26	24.7408	26.31837	42.66677	17.87769	23.28417
6.	6	33	36.05316	36.39048	49.97235	27.25084	26.36919
7.	7	49	49.37368	47.85995	56.14913	41.53828	29.45422
8.	8	68	64.56717	60.6794	61.4997	63.31653	32.53925
9.	9	80	81.49841	74.80914	66.21924	96.51297	35.62427
10.	10	100	100.0322	90.21513	70.44101	147.1141	38.7093
Sum of Deviations			-0.000012	15.73883	15.73885	-18.6549	120.0783
Mean Deviations $\overline{d}$			-0.000001	1.573883	1.573885	-1.86549	12.00783
Standard Deviation σ			1.651121	4.750985	17.37627	23.88992	36.58156

The equations found by the programme:

1. $y = 3.033334 - 2.143551x + 1.409674x^2 + -0.022533x^3$
2. $y = 1.506539x^{1.777299}$
3. $y = 40.069756\ln(x) - 21.823015$
4. $y = 2.172543e^{0.421531x}$
5. $y = 3.085026x + 7.859038$

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HISLOPIA *JOURNAL*	VOL. 3(2)	DECEMBER 2010

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Published by Hislop College, Civil Lines, NAGPUR-440 010. INDIA .
Type Set by: Ameya Computer Centre, Ravinagar Sq.
Amravati Road, Nagpur - 440 001 (India)