



AN INTERACTIVE SOFTWARE FOR CURVE FITTING

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ABSTRACT

An interactive and user friendly software in Visual Basic is presented for obtaining suitable coefficients in curve fitting operations. A general conjugate gradient optimization algorithm (GCG-GSAP) is implemented for fitting curves to existing data. The user supplies up to 100 pairs of data in the form of a worksheet. The program determines values of parameters of a function such that deviations from the given data are minimized. Sum of the squares of the differences is postulated as an optimization criterion, which is assigned as a multi-variant objective function to be minimized.

To start the curve fitting process, the user selects one of a number of available models or their combinations. CurveFit is able to make intuitive identifications, and it is able to determine the best fit for a given set of data, utilizing built-in optimization criteria. The output from the software includes the input data, the corresponding set of calculated values, and the differences between the two sets. Data sets and plots can be printed directly from within CurveFit, or alternatively, they can be exported to Excel for further processing.

Keywords: *coefficients, curve fitting, plotting, regression, software*

1. INTRODUCTION

Engineering data is frequently available exclusively in tabular or graphical form. There seems to be a clear need to develop mathematical models that adequately represent existing data, if this data is to be utilized in computer-aided design or for automation of computations in general. One may cite as an example, the design of full journal bearings and hydrodynamic lubrication, where about 40 Raimondi-Boyd charts [Raimondi and Boyd, 1958] need to be referred to, each chart containing four parameters.

Fitting of smooth curves to data by the aid of a computer has been investigated for many years. To cite a few contemporary research efforts, Adey and associates [Adey et al, 1985] presented a computer program for non-linear curve fitting. They treated the mathematical modeling of data where linear and non-linear parameters are separable, and they applied the minimization technique on the non-linear parameters by the aid of an eigenvalue analysis. Zhou [1990] presented a method for the fitting of smooth curves to noisy data. He represented a curve by two nonlinear functions of arc length. Still other researchers [Baumgart et al, 1991; Webb et al, 1990; Porter et al, 1991; Hood, 1987; Pintelon and Schoukens, 1996; Rosin and West, 1995; Taubin, 1995; Codrington et al, 1994; Conte et al, 1993; Werman and Geyzel, 1995; Kajfez, 1994; Ma et al, 1993; Kanatani, 1994; Fowler and Bartels, 1993; Yamamura, 1993; Gunther and Spot, 1993; Kiryati and Bruckstein, 1992] fitted curves to data, without obtaining equations for the curves.

Splines are piecewise defined curves, each piece belonging to a certain family, generally of polynomial functions. Splines have been extensively used in computer-aided geometric modeling systems. Of these, least-squares spline fitting is utilized in many areas of scientific computation, computer graphics, optical character recognition, and signal/image processing for generating functional representations of sampled data. Thus Flickner and associates [Flickner et al, 1994] described the theory of least squares spline fitting, and provided practical algorithms for the same, with emphasis on 2-D closed curves. Splines were utilized by a number of other researchers [Chou and Piegl, 1992; Yu and Cheng, 1989; Pinkerton, 1992; Safraz, 2000, 2001, 2001a, 2002, 2002a] for curve fitting applications.

An area of intense current activity where spline models are used is that of shape matching and surface modeling. Thus Ferrero and associates [1994] and other researchers [Li et al, 1993] used curve fitting for the characterization of signals. Still others [Pengfei and Chirlian, 1995; Sederberg, 1990] used curve fitting for defining shapes, and for object recognition [Taubin et al, 1994; Rimon and Boyd, 1992; Muir, 1990].

A multi-reference modal parameter identification technique was introduced by Yoshimura [1991]. The method is based on a least squares principle, and utilizes frequency response functions as input data. The author uses the Gauss-Newton method to minimize weighted squared errors. Still

other researchers [Pinkerton et al, 1992; Sachdev and Nagpal, 1991] made use of the least squares technique in their curve fitting work.

In what follows, an interactive and user friendly software is introduced for computer-aided curve fitting, whereby suitable coefficients are obtained for the resulting equations.

2. GCG-GSAP ALGORITHM

Many problems in design can be posed in the form of a general nonlinear problem. While a number of approaches to the solution of such problems have been suggested, the *penalty function transformation* [Carroll, 1961] appears to be the most widely used. Most of the techniques for solving the problem by the penalty approach are either direct search or gradient based (descent). The technique adopted in the present study is a general purpose descent algorithm developed by Johnson and Townsend [1980]. The method is based on a *generalized conjugate direction algorithm* (GCG) that searches for *acceptable points*.

One of the strategies to search for an acceptable point (i.e., a value of λ_k satisfying conditions I, II, and III below) is the so called GSAP after *golden section acceptable point* search:

$$f(\mathbf{x}^k + \lambda_k \mathbf{s}^k) < f(\mathbf{x}^k) \quad (1)$$

$$\|\mathbf{x}^{k+1} - \mathbf{x}^k\| > 0 \quad \text{for all } k \quad (2)$$

$$\text{and} \quad +\mathbf{s}^{k+1}, \mathbf{g}^{k+1}, < 0 \quad (3)$$

where \mathbf{x} = vector of independent design variables

\mathbf{g} = gradient of $f(\mathbf{x})$

\mathbf{s} = search direction vector

λ = step length parameter

k = multivariate iteration number

$\|\mathbf{v}\|$ = Euclidean norm of \mathbf{v}

and $+\mathbf{w}, \mathbf{v}$, = dot product of \mathbf{w} and \mathbf{v}

The GSAP search identifies an acceptable point by comparing function values along the half line originating at \mathbf{x}^k in the direction \mathbf{s}^k . When a bracket on a point which satisfies the conditions is found, a golden section search is employed to reduce the bracket. During this phase, points are tested at user-specified intervals according to conditions 1, 2, and 3. When an acceptable point is identified, the univariate algorithm returns to the main program with the appropriate value for λ_k .

If an acceptable point is not located after some user-specified maximum number of function evaluations, then the univariate search is considered to have failed - either because the search direction was a poor one or because of an overly large initial step length. The policy followed is to exit from the univariate algorithm, reset the parent algorithm, and reduce the initial step length. The search for an acceptable point in the new search direction then proceeds as before. In this way, the univariate algorithm attempts to identify opportune iterations to employ the reset option.

3. PROGRAM DESCRIPTION

The program is initiated by clicking on its icon on the desktop, upon which the *Main Menu* (Fig. 1) with its logo appears. Under the *File* menu are listed the tool items *New*, *Open*, *Save*, *Save as*, *Export to Excel* and *Exit*. Figure 2 shows the *Input Data* form which appears when data is imported by invoking *File / New* or *File / Open*, and then selecting a data file. The latter form provides a table of x - y values, which may be manually edited. If a file extension is not supplied in the *File / Open* or *File / Save* dialog boxes, then the *.eft* extension is automatically added. *CurveFit* saves all data in ASCII format. Data files are located in the *CurveFit* directory by default. Input data does not need to be ordered.

The *Input Data* form further lists the number of data points in the data set, and provides a grid for plotting, whereby it is possible to display the data by utilizing a linear x - y plot (as shown in Fig. 2), or any of a y - $\log x$, x - $\log y$ or a $\log x$ - $\log y$ plot. These choices are indicated at the right edge of the form. Pressing the *Cancel* button on the *Input Data* form enables a return to the original data, whereas opting for the *OK* button signals acceptance of any changes that were made in the data set.

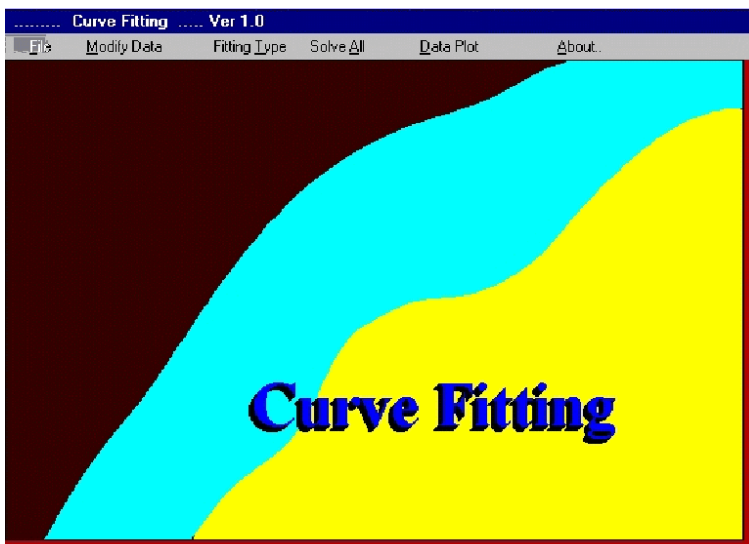


Fig. 1 The main menu of CurveFit.

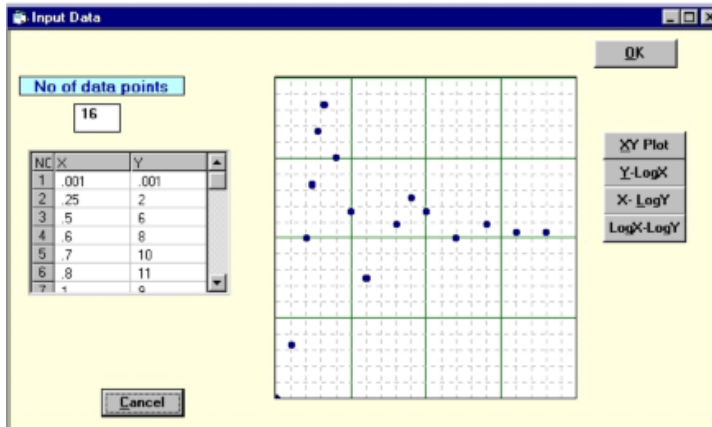


Fig. 2. *Input Data* form.

When *File / Export to Excel* is invoked from the *Main Menu* either before or after curve fitting, *CurveFit* searches for the *Excel* software installed in the host computer, activates it, and then exports the *Input Data* and the *Calculated Data* (if any) to *Excel*.

A second menu item on the *Main Menu* is *Modify Data*, which allows the user to either accept an already open set of (existing) data or to manually modify it. This is accomplished by clicking on *Modify Data*. To *edit* a data point, the user simply clicks the cell that is to be modified, and types in the new data. Whether data is supplied by importing or by modifying existing data, in both cases the *Input Data* form is obtained (Fig. 2). The *About* button presents information on program version and development.

A further menu item on the *Main Menu* is *Fitting Type* which, when clicked, bares a pop-down menu with a number of choices of curve fitting types that are possible. These include *linear*, *quadratic* and *nth order polynomial* fits, for $3 \leq n \leq 7$. Among the other available fits are the *Ezz-Bedawy*, *exponential family*, *power models*, *growth models*, *sinusoidal family*, *yield-density models* and *miscellaneous* other models. The number of fitting types stands currently at 21.

Also on the *Main Menu* the user is given the option of fitting the data to all of the fitting types. This is performed by clicking on the *Solve All* button.

Selecting, on the *Main Menu*, any of the types of fit that are listed under *Fitting Type* yields a table of coefficients (Fig. 3). These represent *Initial Guess Values* for the curve-fit parameters (coefficients) for the selected fit. The coefficients listed under *old* are the values estimated by *CurveFit* for the existing condition. The user is in a position to either accept the guess values listed under *old* or, if he deems it necessary, he can manually enter his own guess values (under *new*) for the coefficients.



Fig. 3. The menu for *Initial Guess Values*.

In either case, pressing *Plot Preview* in the menu for *Initial Guess Values* (Fig. 3) instructs *CurveFit* to immediately present an initial preview of the plot (Fig. 4). It is possible to introduce modifications at this stage by invoking *Modify Initial Guess* at the lower left of the *Plot Preview* screen of Fig. 4, which leads back to the menu for *Initial Guess Values* shown in Fig. 3. Following the entry of the modifications for the coefficients, the user again invokes the *Plot Preview* button to view the effects of the modifications in the screen of Fig. 4.

It may be pointed out that there exists a *Solve* button, located on the top of the menu for *Initial Guess Values* (Fig. 3). Another *Solve* button may be spotted at the bottom of the *Plot Preview* screen (Fig. 4). Clicking on either of the two *Solve* buttons directs *CurveFit* to undertake a full fledged curve fitting operation. The results of the ensuing computations are displayed in the *Output Plot* Screen of Fig. 5.

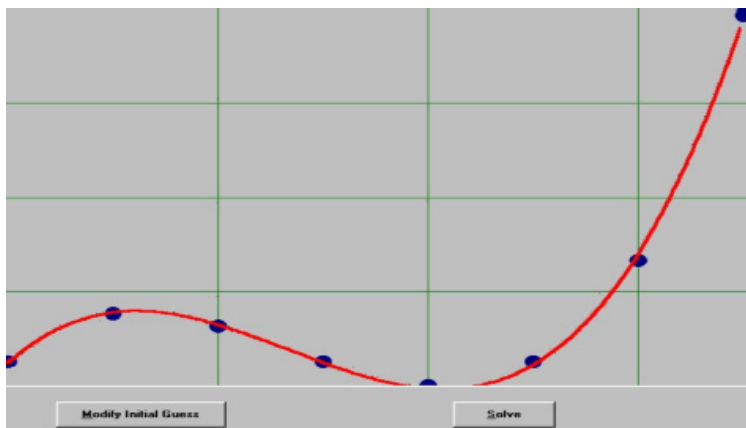


Fig. 4. *Plot Preview* screen.

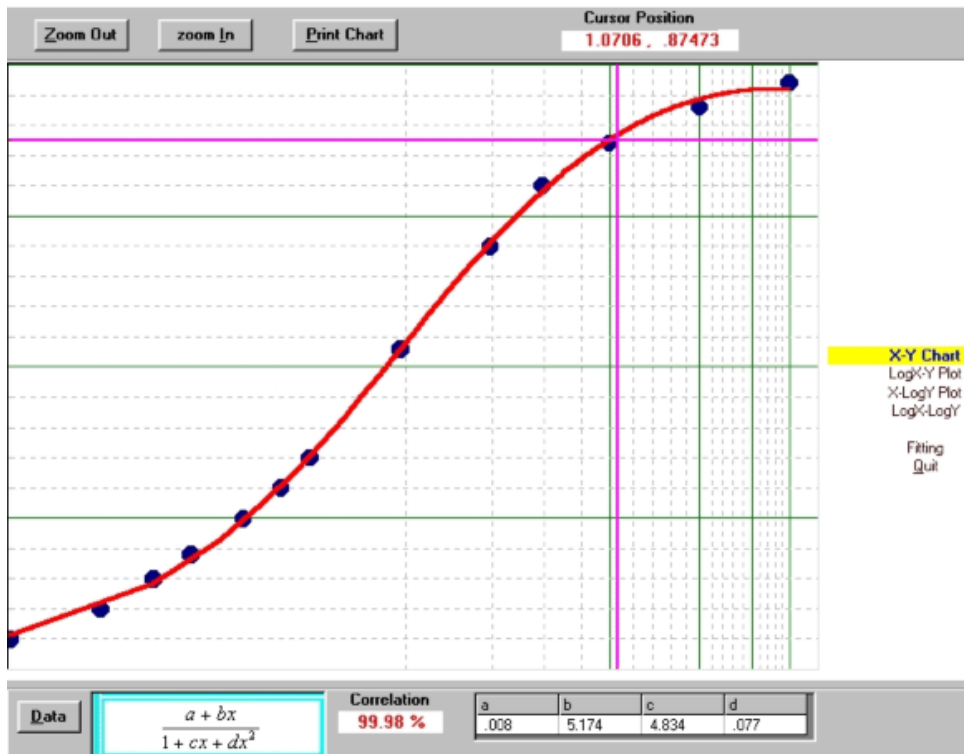


Fig. 5. The *Output Plot* screen.

A number of new features become available in the *Output Plot* screen. These include the *Correlation Constant* (99.98 % for the curve shown), the *Coefficients of the Fit* (expressed as numerical values for *a*, *b*, *c*, and *d* at the bottom of the figure), and the right-hand side of the equation of the fitted function itself in terms of these coefficients. Located to the right of the graph is a list of contact-sensitive display types. By invoking any item in this list, it is possible to display the data and the fit as a linear *x-y* plot, or any of a *y-logx* (shown), *x-logy* or a *logx - logy* plot.

The correlation coefficient is computed by the use of the Spearman rank-order relationship [Press et al, 1992]

$$r_s = \frac{\sum_i (R_i - \bar{R})(S_i - \bar{S})}{\sqrt{\sum_i (R_i - \bar{R})^2} \sqrt{\sum_i (S_i - \bar{S})^2}}$$

where R_i is the rank of x_i among other x 's and S_i is the rank of y_i among the other y 's.

Invoking the *Data* button at the bottom left corner of the *Output Plot* screen leads to the *Data, Residuals and Error Analysis* screen of Fig. 6. The original data (X and Y) is listed in Fig. 6 along with the calculated value Y_c of Y and $D_y = Y - Y_c$. Clicking on the *Error Analysis* button (Fig. 6) causes the opening of yet another (lower) window, where the error at each data point is indicated in the form of a bar chart. Also indicated at the bottom of the latter window are the *mean percentage error*, which is the percentage of $\frac{\sum D_y}{Y_{mean}}$, and the percentage of *dispersion*, which is expressed as, $\frac{\Delta_{max}}{Y_{mean}}$ where Δ_{max} is the maximum of D_y .

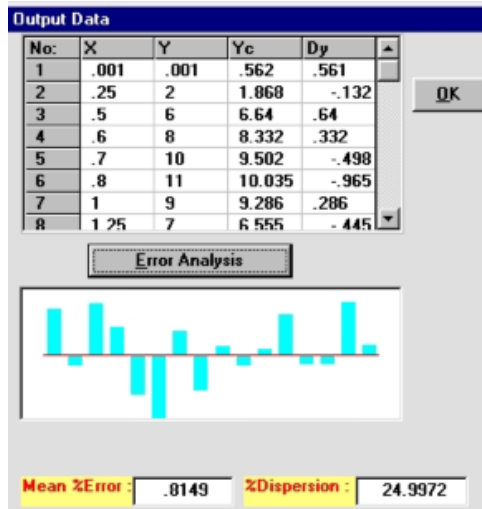


Fig. 6. Screen for *Data, Residuals and Error Analysis*.

Additionally the *Output Plot* screen of Fig. 5 allows *zooming* in and out, by the use of the respective buttons located at the top left of the screen. The instantaneous coordinates of the cursor are also indicated at the top right edge of the *Output Plot* screen.

A further facility that is available in the *Output Plot* screen is the *printing* option. When the *Print Chart* button is clicked, the *Print* screen of Fig. 7 is displayed. Now the user can utilize the facilities offered by *Printer Properties, Configure Port, Connect to Printer, Doc. Properties, Paper Sizes* and *Print* buttons to configure the printer and select the print options before proceeding to print the chart. *CurveFit* actually automatically identifies the printer that is connected to the host computer, and provides the interface for it.

A powerful and novel feature of *CurveFit* is implemented by the actuation of the *Solve All* button. *Solve All* is especially useful when processing data of unknown nature or of undefined best-fit characteristics. When invoked on the *Main Menu*, *Solve All* instructs *CurveFit* to process the given data for all 21 functions in its inventory, and then determines and returns the

Best-Fit as the default display (Fig. 8). It may be verified from Fig. 8 that the *Sinusoidal 3* is at the top of the *ranking list* that is located at the right of the figure, indicating that this function provides the *best fit* for the given data set. In fact this same function is depicted as a plot in the display area at left, and the exact expression for it and its coefficients are exhibited at the bottom of the figure. The correlation coefficient of the fit is observed to be quite satisfactory. The worst fit for the given data set, on the other hand, is the *Modified Exponential* function, which *CurveFit* has placed at the very bottom of the *ranking list*.

The *Plot Preview* area of the *Solve All* screen (Fig. 8) enables rapid visualization of various fits to a given data set. As each regression is completed, an entry appears for it in the *ranking list* on the right of this screen. The *Plot Preview* area is updated every time the data set is changed, reflecting the latest changes in the data set. When solving for polynomials, *Solve All* provides solutions for up to the 4th order, although the order of the polynomial can range from 3 to seven when solving explicitly. Thus the user may wish to invoke the *Data Plot* button on the *Main Menu*, and make use of the resulting *Chart Menu*.

Clicking on an entry in the *ranking list* causes the *Plot Preview* area to generate a graph of that particular regression. In this manner it is possible to manually inspect all fit options that are listed on the *ranking list*. Once the user is satisfied, the user either presses *Esc* or *Quit*, or proceeds to display the selected fit as a linear x - y plot, or as any of a y - $\log x$, x - $\log y$ or a $\log x$ - $\log y$ plot by invoking the *Graph Type* button at the lower right margin of Fig. 8.

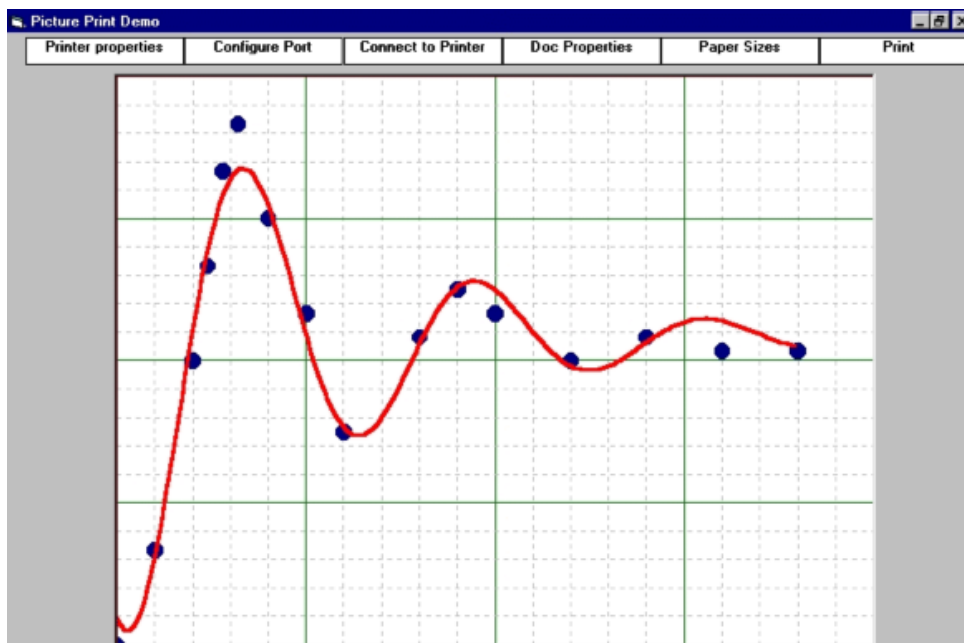


Fig. 7. The *Print* screen of *CurveFit*.

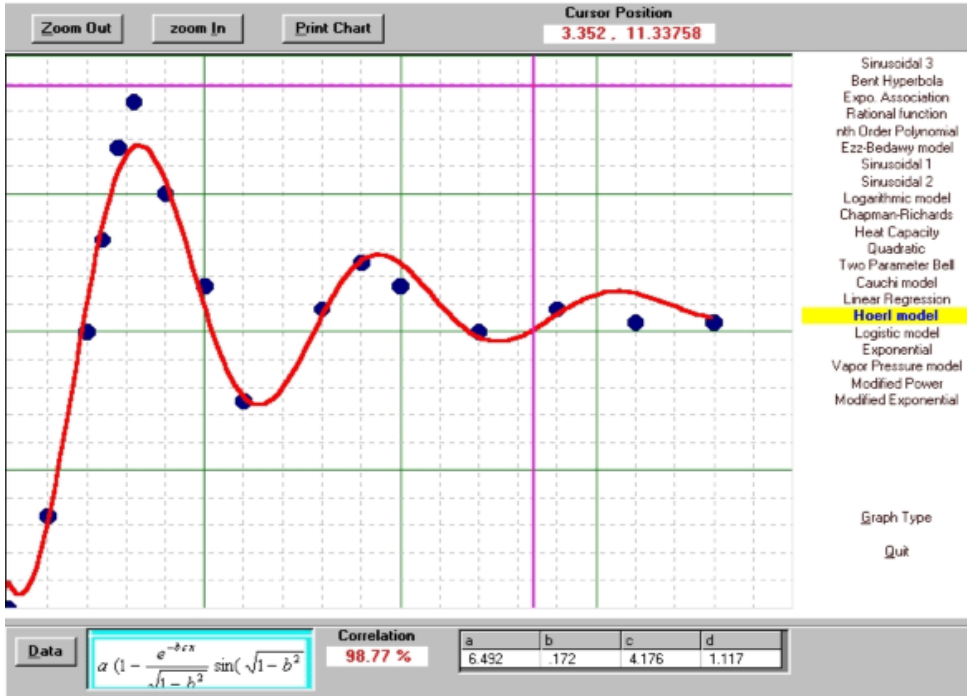


Fig. 8. The *Best Fit* screen of *CurveFit*.

Invoking *Data plot* (on the main menu) after *Solve* leads directly to the *Output plot* screen. *Data plot* is de-activated unless *Solve* is activated a priori. It is possible to *zoom-in* or *zoom-out* on a region in the *Output Plot*. The *zoom* feature is not available on *log* and *semi-log* plots.

It may be pointed out that the *coefficients* of the fit that are displayed at the bottom of the *Output Plot* and the *Best Fit* screens of *CurveFit* relate directly to the physical behavior of the phenomenon that is being modeled. Thus for the plot of Fig.8, where the response of a system with two degrees of freedom is modeled by the (right hand side) of the expression,

$$a \left(1 - \frac{e^{-bcx}}{\sqrt{1-b^2}} \sin(\sqrt{1-b^2} cx + d)\right)$$

where *a* represents the amplitude of the decaying function, *b* is the damping ratio, *c* is the natural frequency and *d* is the phase angle.

4. CONCLUDING REMARKS

CurveFit is a compact (under 1 MB) and comprehensive curve fitting software for Windows, similar to those available with packages like MathCad, Mathematica and Matlab. It implements a toolbox of fitting techniques that currently comprises 21 linear and nonlinear regression models, enabling the precise representation of input data. *CurveFit* employs the GCG-SAP algorithm for quick and robust nonlinear regression performance.

Data input to *CurveFit* can be by simple ASCII data files as well as by manual insertion from within the program. In the case of the former, the software is able to ignore comments and other text. *CurveFit* can print the data set or export the original as well as generated data to *Excel* for further processing.

One powerful feature of *CurveFit* that makes it especially user-friendly is that it is able to examine all possible regression models for a given data set, and determine and report the *best fit*. An internal mechanism keeps track of the fitting performance, and arranges the models from the best to the worst fit. The results are displayed in terms of a *ranking list* and contact-sensitive graphs.

CurveFit features full-featured graphing capabilities, with customizable dynamic graphs that give immediate feedback on the quality of curve fit. The graphs can be copied to the clipboard for use in other Windows applications or printed as hard copies from within *CurveFit* itself. Future developments on the program envisage to further enhance the flexibility and utility of the program by enabling the user to enter user-defined functions from the keyboard.

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