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Introduction

Scientific research often involves the measurement of two sets of variables to determine the functional relationship between the two variables. Because of the nature of experiments, the ordinate variable usually contains random errors. In those instances in which the underlying form of the relationship between the two variables is known, the relationship can be approximately obtained through the use of a mathematical tool such as the method of least squares (ref. 1). If the underlying relationship is unknown or if the relationship is known but is too complicated to be easily computed, the function is often approximated with polynomials and other simple functions.

If the error in the ordinate data is negligible or zero, intermediate values can be calculated by interpolating. Various spline interpolation functions have found widespread use over the years, including cubic splines (ref. 2), basis splines (B-splines) (ref. 3), and splines under tension (ref. 4). The last type of spline was devised to overcome the occasional occurrence of spurious local behavior of the cubic spline. The spline under tension reduces the deviant behavior by applying a constant tension to the cubic spline over the entire data range. The disadvantage to this approach is that the tension is also applied in those regions where the user would be satisfied with an untensioned spline.

A lesser known tension spline developed by Späth (ref. 5), called the "rational spline," allows the user to specify different tension values between each adjacent pair of knots. This is accomplished by introducing into the cubic terms of the spline a denominator containing a different parameter for each knot interval; depending on the parameter value, the rational spline can be made to behave like a cubic or a linear function. In this manner the behavior of the rational spline between each pair of knots can be adjusted by trial and error. Recently, Frost and Kinzel (ref. 6) introduced an automatic adjustment scheme which varies the tension parameter for each interval until the maximum deviation of the spline from the line joining the knots is less than or equal to a user-specified amount. This procedure frees the user from the drudgery of adjusting individual tension parameters while still giving him control over the local behavior of the spline.

If the ordinates of the data contain errors, algorithms are available for finding least-squares approximations by using cubic splines (refs. 7 and 8). Although the cubic-spline approximations provide smooth representations of the data, in some instances the approximations exhibit the same deviation that occurs with interpolating splines. For this reason, a spline approximation method which smooths the data without fluctuating wildly would be a very useful tool.

This paper presents an algorithm for weighted least-squares approximations with rational splines. The algorithm contains the automatic adjustment procedure of Frost and Kinzel (ref. 6) for determining the tension parameters and a constrained weighted least-squares solution comparable to that found in reference 8 for estimating spline coefficients. First, the derivation and description of the algorithm are presented. These are followed by an illustrative example comparing rational-spline and cubic-spline representations of the data.

Derivation of Equations

Let the set of n data points be represented by (x_i, y_i), where $i = 1, 2, \ldots, n$ and $x_1 < x_2 < \ldots < x_n$. (A list of symbols used in this paper appears after the references.) Let w_i (for $i = 1, 2, \ldots, n$) be a set of positive weights indicating confidence in the corresponding ordinate values. Select l knots of the spline, the abscissas are $\bar{x}_k$, where $k = 1, 2, \ldots, l$ and $x_1 = \bar{x}_1 < \bar{x}_2 < \ldots < \bar{x}_{l-1} < \bar{x}_l = x_n$. The ordinates of the knots are $\bar{y}_k$; because the spline will pass through the knots, the knot ordinates are unknown at this point. Also, define $dx_k = \bar{x}_{k+1} - \bar{x}_k$ for $k = 1, 2, \ldots, l-1$ to be the length of each subinterval defined by two consecutive knot abscissas. The rational spline on interval k $(k = 1, 2, \ldots, l-1)$ is defined in references 5 and 6 to be

$$F_k(x) = A_k u + B_k t + C_k \frac{u^3}{P_k t + 1} + D_k \frac{t^3}{P_k u + 1} \qquad (\bar{x}_k \leq x < \bar{x}_{k+1}) \tag{1}$$

where

P_k	tension parameter
A_k, B_k, C_k, D_k	unknown coefficients
u	$= (\bar{x}_{k+1} - x)/dx_k$
t	$= (x - \bar{x}_k)/dx_k = 1 - u$

Equation (1) is defined for all independent variables x in the data range if the tension parameter P_k is restricted to $P_k > -1$. If P_k is set to zero, equation (1) reduces to a cubic-spline function. As P_k increases from zero, the cubic terms decrease and $F_k(x)$ tends to the equation of the line joining the knots at $\bar{x}_k$ and $\bar{x}_{k+1}$. This characteristic of $F_k(x)$ is exploited in the automatic adjustment algorithm devised by Frost and Kinzel (ref. 6) to determine the value of P_k.

Evaluation of equation (1) for each subinterval requires knowledge of the four coefficients A_k, B_k, C_k, and D_k. This means that for l knots (equivalently, $l-1$ subintervals), $4l - 4$ coefficients must be estimated by the method of least squares. The magnitude of the estimation problem can be reduced by writing $F_k(x)$ in terms of the unknown function values

($\bar{y}_k$ for $k = 1, 2, \ldots, l$) and second derivatives ($\bar{y}''_k$ for $k = 1, 2, \ldots, l-1$) at the knots. To do this, first evaluate $F_k(x)$ at the knots $\bar{x}_k$ and $\bar{x}_{k+1}$ and set respective results equal to $\bar{y}_k$ and $\bar{y}_{k+1}$. If $x = \bar{x}_k$, then $u = 1$, $t = 0$, and

$$\bar{y}_k = F_k(\bar{x}_k) = A_k + C_k \tag{2}$$

If $x = \bar{x}_{k+1}$, then $u = 0$, $t = 1$, and

$$\bar{y}_{k+1} = F_k(\bar{x}_{k+1}) = B_k + D_k \tag{3}$$

Next, differentiate $F_k(x)$ in equation (1) twice, evaluate the result at $\bar{x}_k$ and $\bar{x}_{k+1}$, and set respective results equal to $\bar{y}''_k$ and $\bar{y}''_{k+1}$. The second derivative is

$$F''_k(x) = C_k \frac{2P_k^2 u^3 + 6P_k(P_k t + 1)u^2 + 6(P_k t + 1)^2 u}{dx_k^2 (P_k t + 1)^3} + D_k \frac{2P_k^2 t^3 + 6P_k(P_k u + 1)t^2 + 6(P_k u + 1)^2 t}{dx_k^2 (P_k u + 1)^3} \tag{4}$$

Evaluating equation (4) at the knots yields

$$\bar{y}''_k = F''_k(\bar{x}_k) = C_k \frac{2P_k^2 + 6P_k + 6}{dx_k^2} \tag{5}$$

and

$$\bar{y}''_{k+1} = F''_k(\bar{x}_{k+1}) = D_k \frac{2P_k^2 + 6P_k + 6}{dx_k^2} \tag{6}$$

Solving equations (2), (3), (5), and (6) for A_k, B_k, C_k, and D_k yields the relationships

$$A_k = \bar{y}_k - H_k \bar{y}''_k \tag{7}$$

$$B_k = \bar{y}_{k+1} - H_k \bar{y}''_{k+1} \tag{8}$$

$$C_k = H_k \bar{y}''_k \tag{9}$$

$$D_k = H_k \bar{y}''_{k+1} \tag{10}$$

where

$$H_k = \frac{dx_k^2}{2(P_k^2 + 3P_k + 3)} \tag{11}$$

Substituting equations (7) through (11) into equation (1) and rearranging leads to the following rational-spline form:

$$F_k(x) = u\bar{y}_k + H_k \left(\frac{u^3}{P_k t + 1} - u \right) \bar{y}''_k + t\bar{y}_{k+1} + H_k \left(\frac{t^3}{P_k u + 1} - t \right) \bar{y}''_{k+1} \tag{12}$$

Equation (12) shows the direct dependence of the rational spline on the function and the second derivatives at the knots. If P_k is set to zero, equation (12) reduces to the equation of a cubic spline given in reference 8. In this form, only the $2l$ parameters $\bar{y}_k$ and $\bar{y}''_k$ for $k = 1, 2, \ldots, l$ need to be estimated from the data.

Since equation (12) does not explicitly depend on the first derivatives at the knots, there is no assurance that the first derivative is continuous at the interior knots. To overcome this deficiency, the first derivatives must be constrained to be continuous at these knots. The first derivative of equation (12) is

$$F'_k(x) = -\frac{\bar{y}_k}{dx_k} - \frac{H_k}{dx_k}\left[\frac{3u^2(P_k t + 1) + u^3 P_k}{(P_k t + 1)^2} - 1\right]\bar{y}''_k + \frac{\bar{y}_{k+1}}{dx_k} + \frac{H_k}{dx_k}\left[\frac{3t^2(P_k u + 1) + t^3 P_k}{(P_k u + 1)^2} - 1\right]\bar{y}''_{k+1} \tag{13}$$

The continuity constraints to be imposed are

$$F'_k(\bar{x}_{k+1}) = F'_{k+1}(\bar{x}_{k+1}) \qquad (k = 1, 2, \ldots, l-2) \tag{14}$$

Using equation (13) for $F'_k(\bar{x}_{k+1})$ and $F'_{k+1}(\bar{x}_{k+1})$ in equation (14) and rearranging yields the following $l-2$ constraint equation (for $k = 1, 2, \ldots, l-2$):

$$-\frac{\bar{y}_k}{dx_k} + \frac{H_k}{dx_k}\bar{y}''_k + \left(\frac{1}{dx_k} + \frac{1}{dx_{k+1}}\right)\bar{y}_{k+1} + \left[\frac{(P_k + 2)H_k}{dx_k} + \frac{(P_{k+1} + 2)H_{k+1}}{dx_{k+1}}\right]\bar{y}''_{k+1} - \frac{\bar{y}_{k+2}}{dx_{k+1}} + \frac{H_{k+1}}{dx_{k+1}}\bar{y}''_{k+2} = 0 \tag{15}$$

This equation contains the six unknowns y and y'' at the knots $\bar{x}_k$, $\bar{x}_{k+1}$, and $\bar{x}_{k+2}$.

Equation (12) evaluated at the data points along with the constraint equation (15) form the basis for finding a rational-spline approximation. The approximation is found by solving a constrained weighted least-squares problem. In order to solve this problem, the following matrices are defined. Let $\bar{\mathbf{Y}}$ be the $2l$ column vector $\bar{\mathbf{Y}} = (\bar{y}_1, \bar{y}''_1, \bar{y}_2, \bar{y}''_2, \ldots, \bar{y}_l, \bar{y}''_l)^T$, where superscript T indicates matrix transpose. Let E be the $n \times 2l$ matrix containing cofactors of $\bar{y}_k$ and $\bar{y}''_k$ (for $k = 1, 2, \ldots, l$) in equation (12) evaluated at the data abscissas x_i (for $i = 1, 2, \ldots, n$); each row corresponds to one data point. Because the coefficients ($\bar{y}_k, \bar{y}''_k$) change from subinterval to subinterval, the matrix E has the following overlapping block structure:

$$E = \begin{bmatrix} \boxed{\begin{array}{c}\text{Cofactors}\\ \text{of}\\ \text{subinterval } 1\end{array}} & & & \\ & \boxed{\begin{array}{c}\text{Cofactors}\\ \text{of}\\ \text{subinterval } 2\end{array}} & & \\ & & \ddots & \\ & & & \boxed{\begin{array}{c}\text{Cofactors}\\ \text{of}\\ \text{subinterval } l-1\end{array}} \end{bmatrix}$$

Details of the nonzero entries in E (those in the blocks above) are given in appendix A. Let $\mathbf{Y}$ be the $n \times 1$ column vector containing the n data ordinates y_i (for $i = 1, 2, \ldots, n$); then the scalar equation $y_i = F_k(x_i)$ for $\bar{x}_k \leq x_i < \bar{x}_{k+1}$ and $i = 1, 2, \ldots, n$ can be written as the matrix equation

$$\mathbf{Y} = E\bar{\mathbf{Y}} \tag{16}$$

Finally, let W be an $n \times n$ diagonal weight matrix containing the weights w_i (for $i = 1, 2, \ldots, n$) on the diagonal.

The constraint equation (15) can be written in matrix form as

$$S\bar{\mathbf{Y}} = 0 \tag{17}$$

where S is the $l - 2 \times l$ matrix of cofactors of $\bar{y}_k$ and $\bar{y}_k''$ ($k = 1, 2, \ldots, l$) in equation (15). Because equation (15) relates $\bar{y}_k$ and $\bar{y}_k''$ at three consecutive knots, S has the structure

$$S = \begin{bmatrix} x & x & x & x & x & x & 0 & 0 & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & x & x & x & x & x & x & 0 & 0 & \cdot & \cdot & 0 \\ 0 & 0 & 0 & 0 & x & x & x & x & x & x & 0 & \cdot & \cdot \\ \vdots & \vdots & & & & & \ddots & & & & & & \vdots \\ 0 & 0 & \cdot & \cdot & 0 & x & x & x & x & x & x & 0 & 0 \\ 0 & 0 & \cdot & \cdot & 0 & 0 & 0 & x & x & x & x & x & x \end{bmatrix}$$

The nonzero entries in S are defined in appendix A.

With these matrix definitions the constrained least-squares problem requires the minimizing of $(\mathbf{Y} - E\bar{\mathbf{Y}})^T W (\mathbf{Y} - E\bar{\mathbf{Y}})$ with respect to $\bar{\mathbf{Y}}$ such that $S\bar{\mathbf{Y}} = 0$. With $\mathbf{G}$ defined as an $l - 2$ vector of Lagrange multipliers, the constrained problem can be rewritten as the unconstrained problem, minimizing $(\mathbf{Y} - E\bar{\mathbf{Y}})^T W (\mathbf{Y} - E\bar{\mathbf{Y}}) + 2\mathbf{G}^T S\bar{\mathbf{Y}}$ with respect to $\bar{\mathbf{Y}}$ and $\mathbf{G}$. The solutions of this minimization problem (refs. 1 and 8) are

$$\bar{\mathbf{Y}} = [E^T W E]^{-1} E^T W \mathbf{Y} - [E^T W E]^{-1} S^T \mathbf{G} \tag{18}$$

and

$$\mathbf{G} = \left[S[E^T W E]^{-1} S^T\right]^{-1} S[E^T W E]^{-1} E^T W \mathbf{Y} \tag{19}$$

where the superscript -1 denotes a matrix inverse.

For the user interested in a measure of the error in the estimates, the covariance matrix of the constrained estimates in terms of $\bar{\mathbf{Y}}$ is readily calculated with the matrices used in equations (18) and (19). As shown in reference 1, the covariance matrix is

$$V = s^2 \left[E^T W E\right]^{-1} \times \left[I - S^T \left[S \left[E^T W E\right]^{-1} S^T\right]^{-1} S \left[E^T W E\right]^{-1}\right] \tag{20}$$

In equation (20), s^2 is the estimated variance of the measurement error defined by (see refs. 1 and 8)

$$s^2 = \frac{1}{n - 2l} (\mathbf{Y} - E\bar{\mathbf{Y}})^T W (\mathbf{Y} - E\bar{\mathbf{Y}}) \tag{21}$$

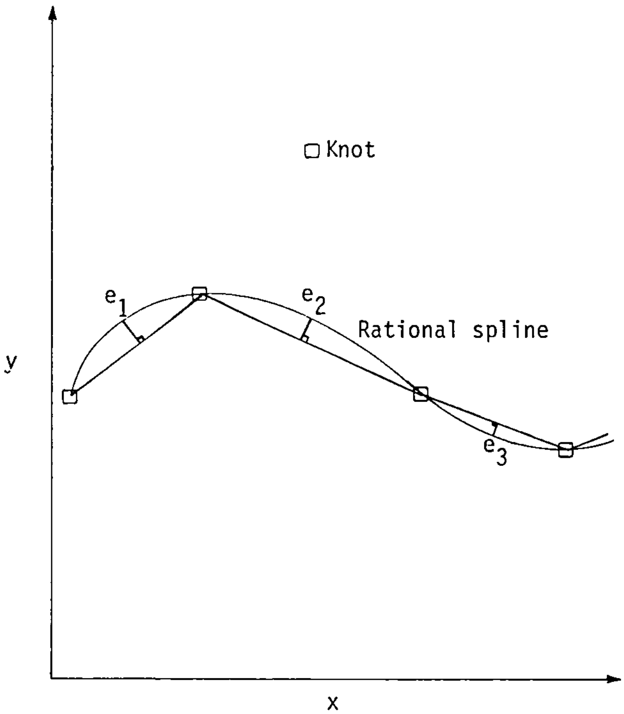

Figure 1. Illustration of maximum deviation of rational spline from line segments joining knots.

Tension Adjustment Algorithm

The Frost and Kinzel tension adjustment algorithm is given below; detailed equations are given in appendix B. The tension adjustment algorithm for interpolation begins by setting all tension parameters P_k to zero and calculating the cubic-spline interpolating function. Each interval is individually tested according to its own criterion to determine if the tension must be adjusted; if additional tension is required, then P_k is incremented by one. For each interval, the criterion to be met is that the maximum deviation e_k of the rational spline from the line segment joining the knots not exceed a user-specified proportion of the length of that line segment. (See fig. 1.) If the maximum deviation exceeds the user-specified value, the tension is increased. Once all the intervals have been tested and appropriate tension parameters incremented, then one of two events occurs. If none of the tension parameters changed, then the procedure is ended; if at least one tension parameter changed, then a new rational spline is calculated and the maximum deviations are tested. The process of calculating the interpolating rational spline, testing maximum deviations, and adjusting tension parameters can be iterated until either no parameter adjustment occurs or a specified number of iterations have been made.

Rational-Spline Approximation Procedure

The constrained weighted least-squares problem is straightforward to solve and requires no iteration. However, because the tension adjustment algorithm is iterative, combining this algorithm with the least-squares solution yields an approximation which must be iterated and is completely analogous to the rational-spline interpolation algorithm.

The approximation procedure consists of the following steps:

1. Initially set all tension parameters P_k to zero.
2. With equations (18) and (19), solve the constrained weighted least-squares problem for the function ($\bar{y}_k$) and the second derivative ($\bar{y}_k''$) values at the knots.
3. Test the maximum deviation of the rational spline in each knot interval; if the maximum deviation exceeds the corresponding user-specified bound, increment the tension parameter by one.
4. If the maximum number of iterations has been tried or if none of the tension parameters have been adjusted, then stop. Otherwise return to step 2 for the next iteration.

The initial pass through step 2 with tension parameter values of zero produces the cubic-spline approximation (ref. 8) to the data. Later iterations gradually tighten the tension to meet the user's criteria. An example is presented in the following section to illustrate the approximation procedure.

The rational-spline approximation algorithm does have two basic limitations. First, in order for the least-squares problem to be well-defined, there must be at least three data points on each interval defined by consecutive pairs of knots. Second, since the tension increases by one during each iteration, the algorithm may require an excessive number of iterations to meet the user-specified criterion of a small deviation. For these cases, in which an essentially linear fit is desired, the user is advised to examine the results of several different large tension values.

Example

The data chosen to illustrate the rational-spline approximation consist of 84 values of terrain elevations taken during a land survey. The measurements were equally spaced at 100-ft intervals and were measured with an accuracy of 0.1 ft.

Nine spline knots were located at the two endpoints of the independent-variable range and at seven intermediate points. The intermediate knots were located at points which appeared to give a reasonable cubic-spline fit. The resulting fit is illustrated in figure 2. The fit is quite poor to the right of the fifth knot (located at $x = 25$); the standard deviation of the fit is 1.43 ft.

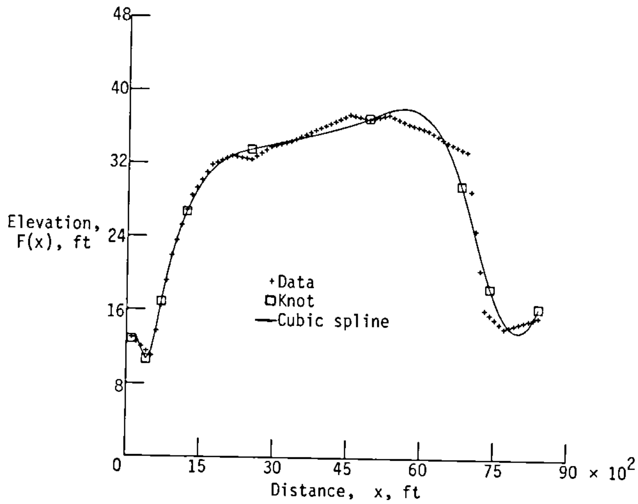

Figure 2. Cubic spline fit to terrain elevation data.

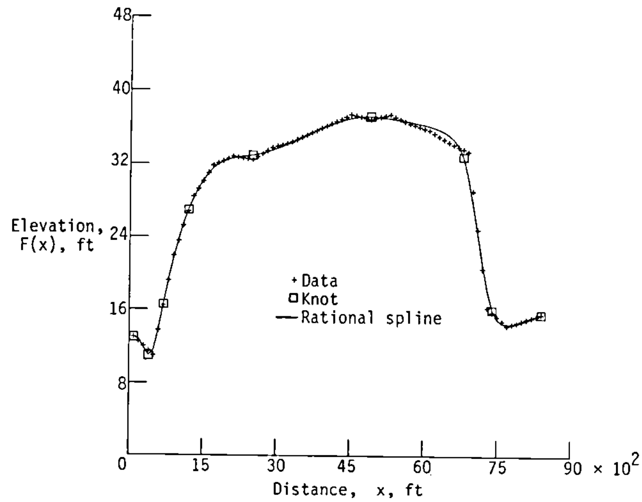

Figure 3. Rational spline fit to terrain elevation data.

One approach to improving the fit is to add knots and to fit a new cubic spline. However, for each knot added, two additional unknowns (function value and second derivative) must be estimated. The fit can be improved without any additional knots by adjusting tension between the knots. For the terrain elevation data, it appeared that adding tension to the intervals to the right of the first, fifth, sixth, and eighth knots could improve the poor fit over those intervals. For the first interval, a fixed tension of 10 was manually selected. For the three remaining intervals, the adjustment algorithm was applied using the allowed deviations from a line given in table I. The results in table I and figure 3 indicate that tension on only the sixth and eighth intervals was required to give a much-improved fit. The standard error of this rational-spline fit was 0.55 ft and required eight iterations.

TABLE I. RATIONAL SPLINE FIT TO TERRAIN ELEVATION DATA

[Eight iterations required]

Knot	Knot abscissa	Tension	Allowed deviation, percent	Tension
1	1.0	10		Fixed
2	4.0	0		Fixed
3	7.0	0		Fixed
4	12.0	0		Fixed
5	25.0	0	15	Adjusted
6	49.0	7	10	Adjusted
7	68.0	0		Fixed
8	74.0	3	20	Adjusted
9	84.0			

Concluding Remarks

An algorithm for obtaining a least-squares approximation to data with a rational spline has been presented. The rational spline combines the advantages of a cubic function having continuous first and second derivatives with the advantages of a function having independently variable tension between consecutive pairs of knots. Application of the method of least squares to the rational spline leads to a flexible, smooth representation of experimental data.

The example presented illustrates the improved fit that can be obtained by approximating with a rational spline rather than with a cubic spline. Also demonstrated in this example are the choices a user has for each consecutive pair of knots: to apply no tension, to apply fixed tension, or to determine tension with a tension adjustment algorithm. Rational-spline approximation also requires the user's judgment in the selection of the number of knots, the knot abscissas, and the allowed maximum deviations from line segments. The selection of these quantities depends on the actual data and on the requirements of a particular application.

The rational-spline approximation algorithm does have two basic limitations. First, in order for the least-squares problem to be well-defined, there must be at least three data points on each interval defined by consecutive pairs of knots. Second, since the tension increases by one during each iteration, the algorithm may require an excessive number of iterations to meet the user-specified criterion of a small deviation. For these cases, in which an essentially linear fit is desired, the user is advised to examine the results of several different large tension values.

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Appendix A

Matrix Definitions

The nonzero entries of the matrices E and S used in the constrained least-squares solution are presented in this appendix. The matrix definitions are based on equations (12) and (15).

Let $\bar{x}_k \leq x_i < \bar{x}_{k+1}$ for $i = 1, 2, ..., n$. Thus, the nonzero entries in row i of matrix E are

$$E_{i,2k-1} = u$$

$$E_{i,2k} = H_k \left(\frac{u^3}{P_k t + 1} - u \right)$$

$$E_{i,2k+1} = t$$

$$E_{i,2k+2} = H_k \left(\frac{t^3}{P_k u + 1} - t \right)$$

where $u = (\bar{x}_{k+1} - x)/dx_k$ and $t = 1 - u$. These entries form the submatrix of E containing cofactors for subinterval k.

The nonzero entries of the $l - 2 \times l$ matrix S are the cofactors in equation (15). Hence, these entries are given by

$$S_{k,2k-1} = -\frac{1}{dx_k}$$

$$S_{k,2k} = \frac{H_k}{dx_k}$$

$$S_{k,2k+1} = \frac{1}{dx_k} + \frac{1}{dx_{k+1}}$$

$$S_{k,2k+2} = \frac{(P_k + 2)H_k}{dx_k} + \frac{(P_{k+1} + 2)H_{k+1}}{dx_{k+1}}$$

$$S_{k,2k+3} = -\frac{1}{dx_{k+1}}$$

$$S_{k,2k+4} = \frac{H_{k+1}}{dx_{k+1}}$$

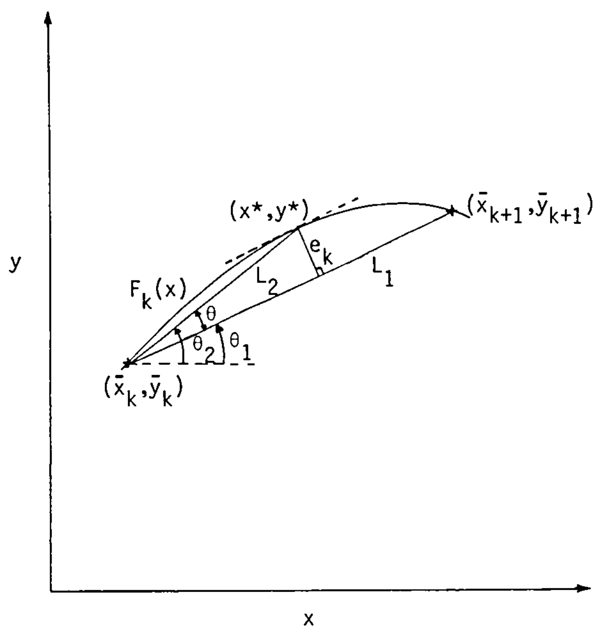
where $k = 1, 2, \ldots, l - 2$.

Appendix B

Equations for Tension Adjustment Algorithm

The derivation and description of the automatic adjustment algorithm are given in this appendix. The description originally given in reference 6 is based on the model given in equation (1). Although the algorithm presented herein is based on the rational-spline definition given in equation (12), the same principle is applied: find the maximum deviation of the rational spline from the line joining the knots.

Consider the knots located at $(\bar{x}_k, \bar{y}_k)$ and at $(\bar{x}_{k+1}, \bar{y}_{k+1})$; the objective is to find the maximum perpendicular distance e_k from the rational spline to the line joining the knots. (See sketch.) The distance between the rational spline and the line is maximized at the point (x^*, y^*) on the rational spline where the derivative of the rational spline is parallel to the line. The slope of the line is given by



$$y_k' = \frac{(\bar{y}_{k+1} - \bar{y}_k)}{(\bar{x}_{k+1} - \bar{x}_k)} = \frac{dy_k}{dx_k} \tag{B1}$$

The line and the derivative of the rational spline are parallel if the slopes are equal, that is, if

$$F_k'(x) = \frac{dy_k}{dx_k} \tag{B2}$$

Substituting equation (13) into equation (B2) and rearranging yields

$$- \bar{y}_k - H_k \left[\frac{3u^2 \left(P_k t + 1\right) + u^3 P_k}{\left(P_k t + 1\right)^2} - 1 \right] \bar{y}_k'' + \bar{y}_{k+1}$$
$$+ H_k \left[\frac{3t^2 \left(P_k u + 1\right) + t^3 P_k}{\left(P_k u + 1\right)^2} - 1 \right] \bar{y}_{k+1}'' - dy_k = 0$$

We can substitute $u = 1 - t$ to obtain

$$- \bar{y}_k - H_k \left[\frac{3(1-t)^2 \left(P_k t + 1\right) + (1-t)^3 P_k}{\left(P_k t + 1\right)^2} - 1 \right] \bar{y}_k''$$
$$+ \bar{y}_{k+1} + H_k \left\{ \frac{3t^2 \left[P_k(1-t) + 1\right] + t^3 P_k}{\left[P_k(1-t) + 1\right]^2} - 1 \right\} \bar{y}_{k+1}''$$
$$- dy_k = 0 \tag{B3}$$

Equation (B3) can be solved for $t (0 \le t \le 1)$ by any one of several iterative methods. One of the simplest methods, the secant method (ref. 9), converges to the appropriate zero (t^*) in just a few iterations.

After t^* is found, the definition of t is used to relate x^* to t^* as follows:

$$t^* = \frac{(x^* - x_k)}{dx_k}$$

or

$$x^* = x_k + t^* dx_k$$

Thus, the ordinate of the point of maximum deviation is given by

$$y^* = F_k(x^*)$$

Now, let $M_1 = y_k'$ and L_1 be the slope and length, respectively, of the line joining the knots; let $M_2 = (y^* - \bar{y}_k)/(x^* - \bar{x}_k)$ and L_2 be the slope and length, respectively, of the line joining $(\bar{x}_k, \bar{y}_k)$ and (x^*, y^*). (See sketch.) Since $M_1 = \tan\theta_1$ and $M_2 = \tan\theta_2$, the angle between the two lines $\theta = \theta_2 - \theta_1$ can be found from

$$\begin{aligned} \tan\theta &= \tan(\theta_2 - \theta_1) \\ &= \frac{\tan\theta_2 - \tan\theta_1}{1 + \tan\theta_1 \tan\theta_2} \\ &= \frac{M_2 - M_1}{1 + M_1 M_2} \end{aligned}$$

Finally, the maximum deviation e_k is given by

$$e_k = L_2 \sin\theta$$

where

$$L_2 = \left[\left(x^* - \bar{x}_k\right)^2 + \left(y^* - \bar{y}k\right)^2 \right]^{1/2}$$

To use the algorithm, let the user-specified criterion be a percent of the length L_1. Then, if $100 e_k / L_1$ is less than or equal to the user-specified percent, P_k does not need to be adjusted; however, if $100e_k/L_1$ is larger than the user-specified percent, then P_k is incremented by one and an additional iteration of the least-squares algorithm is required. The least-squares algorithm is iterated until user-specified criteria are met on all the knot intervals.

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Symbols

A_k, B_k, C_k, D_k	coefficients of rational spline on interval k
dx_k	difference between abscissas of knots defining interval k
dy_k	difference between ordinates of knots defining interval k
E	matrix of cofactors in rational spline
e_k	maximum deviation of rational spline from line for interval k
$F(x)$	rational spline over entire data set
$F_k(x)$	rational spline on interval k
$\mathbf{G}$	vector of Lagrange multipliers
I	identity matrix
L_1, L_2	lengths of lines
l	number of knots
M_1, M_2	slopes of lines
n	number of data points
P_k	tension parameter of rational spline on interval k
S	matrix of cofactors in constraint equation
s^2	estimated variance of measurement error
t, u	variables used to define rational spline
V	covariance matrix of estimates
W	diagonal matrix of weights
w	weight
x	independent variable
x_i	ith abscissa of data
$\bar{x}_k$	abscissa of kth knot
$\mathbf{Y}$	column vector containing ordinates of data
$\bar{\mathbf{Y}}$	column vector containing ordinates of data and second derivatives at knots
y	dependent variable
y_i	ith ordinate of data
$\bar{y}_k$	ordinate of kth knot
$\theta, \theta_1, \theta_2$	angles used in calculating maximum deviation of rational spline from line

Subscripts:

i	ith data point
k	quantity at kth knot

Superscripts:

T	matrix transpose
-1	matrix inverse
$*$	quantity at point on rational spline having maximum deviation from line

A bar over a quantity denotes that quantity at a knot. A prime indicates first derivative with respect to the independent variable. A double prime indicates second derivative with respect to the independent variable.

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16. Abstract

An algorithm for weighted least-squares approximation with rational splines is presented. A rational spline is a cubic function containing a distinct tension parameter for each interval defined by two consecutive knots. For zero tension, the rational spline is identical to a cubic spline; for very large tension, the rational spline is a linear function. The approximation algorithm incorporates an algorithm which automatically adjusts the tension on each interval to fulfill a user-specified criterion. Finally, an example is presented comparing results of the rational spline with those of the cubic spline.

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