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Author
Young, Jonathan D.

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UNIVERSITY OF CALIFORNIA
Lawrence Radiation Laboratory
Berkeley, California 94720

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SMOOTHING DATA WITH TOLERANCES BY USE OF LINEAR PROGRAMMING

Jonathan D. Young

Lawrence Radiation Laboratory
University of California
Berkeley, California 94720

ABSTRACT

This report describes a method for smoothing observed data when the values of the dependent variable are assumed to lie within specified tolerance of the observed value. Linear programming is employed to obtain optimal smoothing of the (local) degree desired within the restraints imposed by the tolerances. First- and third-degree smoothing are discussed, but the method may be extended to higher order.

I. INTRODUCTION

A function f of t has been measured for n distinct and increasing values, t_i, providing f_i^*. The t_i need not be uniformly spaced. For each i, it is assumed that the true value f_i for f lies within some specified tolerance of the measured value f_i^*. That is, the measured value f_i^* may be too large by a quantity d_i^- or too small by a quantity d_i^+, with d_i^- and d_i^+ greater than or equal zero:

$$f_i \geq f_i^* - d_i^- \quad \text{for } i = 1 \cdots n;$$

$$f_i \leq f_i^* + d_i^+ \quad \text{for } i = 1 \cdots n.$$

The tolerances, d_i^- and d_i^+, need not be uniform for the various i and may be zero for some i. This freedom is compatible with measurements known to be more precise at some points than at others. It is also consistent for measurements known to be maximum or minimum values of f at some of the t_i.

Milne[1] proposes smoothing the data, (f_i^*, t_i) for $i = 1 \cdots n$ to obtain f_i by computing a polynomial of degree $m < n$ by the method of least squares. The "smoothed" values, f_i, are then the values of the polynomial at the points t_i. For data for which tolerances are uniform and equal in each direction,

$$d_i^- = d_{i+1}^- \quad \text{for } i = 1 \cdots n - 1;$$

$$d_i^- = d_i^+ \quad \text{for } i = 1 \cdots n;$$

then for some degree, m, the values of f_i obtained will lie within tolerance. This is certainly true for $m = n - 1$, in which case the polynomial is an exact fit for (f_i^*, t_i). In practice, we might seek the least m for which all tolerances are met. For tolerances that are nonuniform (but still equal in each direction at each t_i), the errors at each t_i can be weighted in effecting the least-square fit, thereby adjusting the fit to suit the tolerance. The difficulty of nonequal tolerances can be handled by first moving f_i^* to the midpoint of the allowable variation, obtaining

$$f_i^{**} = f_i^* + \frac{d_i^+}{2} - \frac{d_i^-}{2} .$$

The least-square fit will then assume that f_i^{**} is the most preferred value for f_i, which may or may not be true. If the required degree m to achieve fit within tolerance is relatively large, the values f_i obtained may be based on more inflection in the curve for f(t) than the observer with some a priori knowledge will accept. Interpolation using the least-square polynomial often provides evidence of such inflection. Thus the very globality whereby the change $f_i^* \rightarrow f_i$ is affected by all (t_i, f_i^*) may produce unacceptable results for some data.

In contrast to the least-square polynomial smoothing is the filter method described by Hamming.[2] He sets

$$f_i = \sum_{i=1}^{n} a_j f_j^*, \text{ with } \Sigma a_j = 1 ,$$

and requires $a_j = 0$ except for a few indices near and including i. For example, for uniformly spaced t, we might set

$$f_1 = (5f_1^* + 2f_2^* - f_3^*)/6$$

$$f_i = (f_{i-1}^* + f_i^* + f_{i+1}^*)/3, \qquad \text{for } i = 2 \cdots n-1.$$

$$f_n = (-f_{n-2}^* + 2f_{n-1}^* + 5f_n^*)/6,$$

This choice of coefficients, a_j, is derived from the least-squares first-degree approximation over three points described by Hildebrand,[3] who also gives formulas for third- and fifth-degree approximations over five and seven points respectively. Obviously the filter method is "local", since only f_i^* and a few nearby values affect the resulting f_i. Some global effect may be introduced by repeating the smoothing process on the new values.

For nonuniform steps in t, the coefficients a_j above may be appropriately modified. In general, odd-degree fits are used due to the resulting symmetry in the formulation for interior points. In general, the higher the degree the less smoothing will take place, in fact for degree n-1, there will be no smoothing, since the polynomial will be an exact fit of the data. Without tolerances, the choices of degree (perforce less than n-1) and the number of iterations of the smoothing are subjective, possibly based on a priori knowledge of the behavior of f. Iteration of the smoothing process with approximation of degree m on m+2 points results in the limit in a polynomial of degree m for the whole set of data, which may or may not be desirable.

When tolerances are specified one might choose the least degree-point approximation so that after one smoothing the values f_i remain within tolerance. One might iterate the smoothing as long as the resulting values remain within tolerances. As an alternative a higher degree-point approximation might be employed, again with (presumably more) iterations on the smoothing. The end sought is a proper balance between local and global effect, which is a subjective (possibly well-founded) decision. A practical consideration is the amount of computation involved, which is less for a lower degree.

In the problem of constructing an interpolating function for f based on (t_i, f_i) for i = $1 \cdots n$, valid for the whole interval $(t_1 \cdots t_n)$, a good balance between local and global effects may often be attained by employing the cubic spline fit.[4] This function s(t), defined on $(t_1 \cdots t_n)$, is made up of cubic (in t) arcs defined on $(t_i \ldots t_{i+1})$, where $i = 1 \cdots n-1$, with the requirements of $s_i(t_i) = f_i$ and the matching of first and second derivatives of the left and right cubic segments at each interior point t_i, where $i = 2 \ldots n-1$. Since successive cubics are, in general, distinct, the function s will not possess a third derivative at the interior points, t_i with $i = 2 \ldots n-1$. At these points we have left and right third derivatives which are not, in general, equal. We may use magnitudes of the differences between left and right third derivatives as a measure of the discrepancy of the fit.

For $n \geq 5$, when it is intended to use the cubic spline as the interpolating function on the smoothed values (t_i, f_i), it seems obvious that third-degree five-point approximations should be used in the smoothing process, since this will reduce the discrepancy of the cubic spline fit. Iteration will reduce the discrepancy and in the limit eliminate it. The latter result may or may not be desirable, dependent on whether a priori knowledge indicates that f is in truth "nearly" a cubic. Of course, if f were known to be a cubic we could employ the least-square cubic (as described earlier) for the whole data set (t_i, f_i^*).

When tolerances are imposed, the values f_i obtained by the third degree five-point approximation may lie within these tolerances and we can interate the smoothing as long as resulting values f_i are still acceptable. On the other hand, some or all of the f_i may fall outside tolerance at the first smoothing and third-degree five-point approximation cannot be used. Rather than going to a higher-degree approximation, it now seems desirable to devise a smoothing process as near the third-degree five-point approximation as possible while still obtaining smoothed values, f_i, within tolerance.

II. MIN-MAX SMOOTHING

We first consider a problem, similar to but simpler than that posed in the preceding section. For a set of data $(t_i, f_i^*, d_i^-, d_i^+)$ with $i = 1 \cdots n$ for $n \geq 3$ we wish to find a smoothed set, (t_i, f_i) so that for $j = 2 \cdots n-1$ the f_{j-1}, f_j, and f_{j+1} lie "nearly" on a straight line but

$$\left.\begin{aligned} f_i &\geq f_i^* - d^- \\ f_i &\leq f_i^* + d_i^- \end{aligned}\right\} \quad \text{with } i = 1 \cdots n.$$

We can employ the first-degree three-point approximation described earlier, and if the smoothed values lie within tolerance, we can iterate the smoothing as long as new results still remain within tolerance. On the other hand, if the first smoothing yields values of f_i outside tolerance, this method cannot be employed. (Even if it could be the method below would give an equivalent result.)

We let $h_i = t_{i+1} - t_i$ with $i = 1 \cdots n-1$. The spacing need not be uniform. If we had f_{j+1}, f_j, and f_{j+1} on a straight line we should have

$$(f_{j+1} - f_j)/h_j - (f_j - f_{j-1})/h_{j-1} = 0$$
$$\text{with } j = 2 \cdots n-1.$$

Since this may not be possible we set

$$\frac{1}{h_j} f_{j+1} - \left(\frac{1}{h_j} + \frac{1}{h_{j-1}}\right) f_j + \frac{1}{h_{j-1}} f_{j-1}$$
$$= \epsilon_j \qquad \text{with } j = 2 \cdots n-1,$$

and let $f_\epsilon = \max \left|\epsilon_j\right|$. We try to choose f_i with $i = 1 \cdots n$ in such a way that f_ϵ is minimized. As restraints, we have

$$\left.\begin{aligned} &\frac{1}{h_{j-1}} f_{j-1} - \left(\frac{1}{h_j} + \frac{1}{h_{j-1}}\right) f_j + \frac{1}{h_j} f_{j+1} + f_\epsilon \geqslant 0 && (1)\\ &\text{and}\\ &\frac{1}{h_{j-1}} f_{j-1} + \left(\frac{1}{h_j} + \frac{1}{h_{j-1}}\right) f_j - \frac{1}{h_j} f_{j+1} + f_\epsilon \geqslant 0 && (2) \end{aligned}\right\} j = 2 \ldots n-1$$

and

$$\left.\begin{aligned} f_j &\geqslant f_j^* - d_i^- && (3)\\ -f_j &\geqslant -f_j^* - d_i^+ && (4) \end{aligned}\right\} \text{with } j = 1 \ldots n$$

This linear model has the form (with $f_\epsilon \equiv f_{n+1}$)

$$\text{Minimize } w = \vec{b}\vec{f},$$
$$\text{Subject to linear restraints}$$
$$B\vec{f} \geqslant \vec{c},$$

where $\vec{b}$ and $\vec{f}$ are vectors with n+1 components ($b_i = 0$ with $i = 1 \cdots n$ and $b_{n+1} = 1$), $\vec{c}$ is a vector with 4n - 4 components, and B is a matrix with 4n - 4 rows and n+1 columns.

The model always has a solution, since $f_\epsilon \geqslant 0$, and in the absence of any other nonzero solution we could set $f_j = f_j^*$ and obtain a finite solution

$$f_\epsilon = \max_{j=2 \cdots n-1} \left|\frac{1}{h_j} f_{j+1}^* - \left(\frac{1}{h_j} + \frac{1}{h_{j-1}}\right) f_j^* + \frac{1}{h_{j-1}} f_{j-1}^*\right| \equiv f_\epsilon^*.$$

If $f_\epsilon^* = 0$, then all the points, $(x_j ; f_j^*)$ with $j = 1 \cdots n$ lie on a straight line and no smoothing is needed. Otherwise there is a solution

$$f_j^* - d_j^- \leqslant f_j \leqslant f_j^* + d_j^* \quad \text{with } j = 1 \cdots n,$$
$$0 \geqslant f_\epsilon \leqslant f_\epsilon^*,$$

with f_ϵ having a minimum value. The solution may not be unique, that is, the minimum value of f may be attained for more than one set of values for the f_j with $j = 1 \cdots n$.

The linear model described above is not a linear program, since we cannot restrict the f_j with $j = 1 \cdots n$ to nonnegative values. However, the dual of the above model has the form

$$\text{Maximize} \quad z = cy$$

Subject to

$$Ay = b$$

and

$$y_i \geq 0 \text{ with } i = 1 \cdots 4n-4,$$

where A is the transpose of B and y is the (formal) dual variable vector with 4n -4 components.[5]

The dual model is a linear program and can be solved by the Simplex Algorithm.[6] By the duality theorem we have

$$f_\epsilon = \text{Min } w = \text{Max } z.$$

The algorithm also provides us with the corresponding optimal values for the dual variables of the linear program, and these are the values of f_j with $j = 1 \cdots n$ desired.

Having achieved the above result and remembering that the solution may not be unique, we may seek that "super"-optimal solution for which f_ϵ is minimized and the maximum magnitude of the differences between f_j and f_j^* is minimized.

Suppose that from the previous solution we have

$$\min f_\epsilon = f_\epsilon^{**},$$

then we add to our former restraint matrix B

$$f_\epsilon \geq f_\epsilon^{**} \;,$$

$$-f_\epsilon \geq -f_\epsilon^{**},$$

and letting $f_\delta = \max \left| f_j - f_j^* \right|$ with $j = 1 \cdots n$, we add further

$$f_j + f_\delta \geq f_j^* \;,$$

$$-f_j + f_\delta \leq - f_j^* \;,$$

and take as a new objective

$$\text{Minimize} \quad w = f_\delta \;.$$

we then dualize the linear model to obtain the linear program and solve by the Simplex Algorithm. The dual solution will now give us values for f_j with $j = 1 \cdots n$ for which f_ϵ is minimum and for which f_δ is minimum.

We now extend the method to third degree.

III. THIRD DEGREE MIN-MAX SMOOTHING

For data, (t_i, f_i, d_i^-, d_i^+) with $i = 1 \cdots n$ and $n \geq 5$, we seek smoothed values, f_i, so that for $j = 3 \cdots n-2$ the f_{j-2}, f_{j-1}, f_j, f_{j+1}, and f_{j+2} lie "nearly" on a cubic arc with

$$\left.\begin{array}{l} f_j \geq f_i^* - d_i^- \\ f_i \leq f_i^* + d_i^+ \end{array}\right\} \quad \text{with } i = 1 \cdots n$$

The third-degree five-point approximation may yield values within the specified tolerance, and we shall have:

$$\frac{1}{q_{j-1}} \left\{ \frac{1}{p_j} \left[\frac{f_{j+2}}{h_{j+1}} - \left(\frac{1}{h_{j+1}} + \frac{1}{h_j} \right) f_{j+1} + \frac{f_j}{h_j} \right] - \frac{1}{p_{j-1}} \left[\frac{f_{j+1}}{h_j} - \left(\frac{1}{h_j} + \frac{1}{h_{j-1}} \right) f_j + \frac{f_{j-1}}{h_{j-1}} \right] \right\}$$
$$- \frac{1}{q_{j-2}} \left\{ \frac{1}{p_{j-1}} \left[\frac{f_{j+1}}{h_j} - \left(\frac{1}{h_j} + \frac{1}{h_{j-1}} \right) f_j + \frac{f_{j-1}}{h_{j-1}} \right] - \left[\frac{1}{p_{j-2}} \quad \frac{1}{h_{j-1}} - \frac{1}{h_{j-1}} + \frac{1}{h_{j-2}} \quad f_{j-1} + \frac{f_{j-2}}{h_{j-2}} \right] \right\}$$

$$\epsilon_j = 0 \quad \text{with } j = 3 \cdots n-2,$$

where

$$q_i = h_i + h_{i+1} + h_{i+2}$$

and

$$p_i = h_i + h_{i+1}.$$

However, it may not be possible to obtain $\epsilon_j = 0$ for all j, within the tolerances imposed. We set

$$f_\epsilon = \max \left| \epsilon_j \right| ,$$

as before, and seek to minimize f_ϵ.

We replace the restraints (1) and (2) of the preceding section, respectively, by

$$\alpha_{j-2} f_{j-2} + \alpha_{j-1} f_{j-1} + \alpha_j f_j + \alpha_{j+1} f_{j+1} + \alpha_{j+2} f_{J=2} + f_\epsilon \geqslant 0 \qquad (5)$$

and

$$-\alpha_{j-2} f_{j-2} - \alpha_{j-1} f_{j-1} - \alpha_j f_j - \alpha_{j+1} f_{j+1} - \alpha_{j+2} f_{j+2} + f_\epsilon \geqslant 0, \qquad (6)$$

where

$$\alpha_{j-2} = \frac{1}{q_{j-2}} \cdot \frac{1}{p_{j-2}} \cdot \frac{1}{h_{j-2}} ,$$

$$\alpha_{j-1} = \frac{1}{q_{j-1}} \cdot \frac{1}{p_{j-1}} \cdot \frac{1}{h_{j-1}} - \frac{1}{q_{j-2}} \left[\frac{1}{p_{j-1}} \quad \frac{1}{h_{j-1}} + \frac{1}{p_{j-2}} \left(\frac{1}{h_{j-1}} + \frac{1}{h_{j-2}} \right) \right]$$

$$\alpha_j = \frac{1}{p_{j-1}} \left[\frac{1}{p_j} \cdot \frac{1}{h_j} + \frac{1}{p_{j-1}} \left(\frac{1}{h_j} + \frac{1}{h_{j-1}} \right) \right] + \frac{1}{q_{j-2}} \left[\frac{1}{p_{j-1}} \left(\frac{1}{h_j} + \frac{1}{h_{j-1}} \right) + \frac{1}{p_{j-2}} \cdot \frac{1}{h_{j-1}} \right]$$

$$\alpha_{j+1} = \frac{1}{q_{j-1}} \left[\frac{1}{p_j} \left(\frac{1}{h_{j+1}} + \frac{1}{h_j} \right) + \frac{1}{p_{j-1}} \cdot \frac{1}{h_j} \right] - \frac{1}{q_{j-2}} \cdot \frac{1}{p_{j-1}} \cdot \frac{1}{h_j}$$

$$\alpha_{j+2} = \frac{1}{q_{j-1}} \cdot \frac{1}{p_j} \cdot \frac{1}{h_{j+1}} .$$

The restraints (3) and (4) are retained, and thereafter the procedure is analogous to that outlined in Section II.

The min-max method can be extended to higher degree, but the complexity of the information and size of the linear program model makes this undesirable unless required by a priori knowledge of the behavior of f. It should be noted that restraints (5) and (6) can be greatly simplified in the case of uniform steps in t. We redefine

$$f_\epsilon = h^3 \max \left| \epsilon_j \right|$$

and obtain

$$1/6\, f_{j-2} - 2/3\, f_{j-1} + f_j - 2/3\, f_{j+1} + 1/6\, f_{j+2} + f_\epsilon \geqslant 0 \qquad (5')$$

and

$$-1/6\, f_{j-2} + 2/3\, f_{j-1} - f_j + 2/3\, f_{j+1} - 1/6\, f_{j+2} + f_\epsilon \geqslant 0. \qquad (6')$$

REFERENCES

1. W. E. Milne Numerical Calculus (Princeton University Press, Princeton, New Jersey, 1949), pp. 275-276.

2. R. W. Hamming, Numerical Methods for Scientists and Engineers (McGraw-Hill Book Company, New York, 1962), pp. 314-315.

3. F. B. Hildebrand, Introduction to Numerical Analysis (McGraw-Hill Book Company, New York, 1956), pp 295-296.

4. G. Birkhoff, and C. R. deBoor, Piecewise Polynomial Interpolation and Approximation, in Approximation of Functions, H. L. Garabedian, Ed, (Elsevier Publishing Company, Amsterdam, 1965), pp. 164-168.

5. S. I. Gass, Linear Programming (McGraw-Hill Book Company, New York, 1958).

6. G. B. Dantzig, Rand Report P-89, The Rand Corporation, Santa Monica, California, 1956.

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