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Summary Value Smoothing of Physical Time Series with Unequal Intervals

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An algorithm SUMMOOTH for smoothing raw observations that are unequally spaced is explained. The process generalizes the method of summary values introduced into geophysics by H. Jeffreys. Smoothed data points, defined as the intersection of the local linear and parabolic least-squares fits, are computed for overlapping intervals rather than fixed sequential intervals as in previous work. A new feature is the parallel computation of (smoothed) summary gradients, essential for the Herglotz velocity integration. The interval selection is objective because the position of the smoothed values at each stage depends only on the spacing of the raw sample points. Selection of the starting interval can be made objective by addition of a principle, such as symmetry, or a rule, such as the fitted local curvature must never exceed a fixed value. In practice, selection should employ a trade-off curve between resolution and variance. An advantage of the process is that uncertainties at the summary points are independent. A comparison is given, for scarce data of Mossbauer spectra, with the smoothing method of Talmi and Gilat. Application to ragged time series for v_p/v_s observations in earthquake prediction studies and to the construction of seismological travel-time curves illustrates the value of the method in geophysics.

1. INTRODUCTION

The related processes of smoothing, trend elimination, and interpolation [1] still cause difficulties in the treatment of observed time series. Standard smoothing methods only apply precisely to equally-spaced samples and unequally-spaced data produce unknown fluctuating correlations between the estimated parameters [2] Thus, in both the usual least-squares curve fitting, such as cubic splines, and the operation of a running mean, fluctuations in the data density along the time axis introduce essentially varying weights of undetermined magnitude. Further, the smoothed points have, in general, covariances of significant magnitudes.

Although the problem arises in all fields of data processing, many important illustrations are found in physics and geophysics. In seismology, for example, the most common requirement [3] has been the smoothing of observed travel times T of

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seismic waves as a function of transmission distance Δ. In order to derive the corresponding velocities along the path, an inverse functional that contains derivatives $dT/d\Delta$ is used. Thus, subjective selection of a smoothing process often determines the form of the velocity variation. More recently, physical parameters associated with earthquake occurrence have been plotted against time in an attempt to detect trends which might be forerunners of impending major earthquakes [4]. Here, subjectivity in the smoothing procedures can introduce fallacious inferences because the prediction is made from the form of the smoothed series at the (most recent) end of the range.

The method explained in this paper is based on the method of summary values developed by Jeffreys [5] in a seismological context. The method applies to both dense and scarce data in the presence of random errors when no definite functional form is known. In such cases it must be suspected a priori that the form of the curve changes radically from one end of the range to the other. In other words, a smoothed value must be obtained from the observations in its immediate neighborhood rather than over the whole range as is often done with disastrous consequences in primitive least-squares curve fitting. As previously formulated, the method of summary values simply selects a convenient subrange as standard interval. Linear and quadratic forms are then fitted by least squares in each interval. The summary points are the intersections of the two curves which, of course, may always be computed. At each such point it may be shown that the uncertainties of the estimated values are independent [6]. The summary points, therefore, not only give the linear trend in each range, but also take account of the local parabolic curvature.

Summary value smoothing is also a valuable tool in estimation of the smooth gradients (or derivative curve) of the time series. The argument, apparently previously overlooked, is as follows: The summary linear trend in an interval is the slope of the linear form. However, this slope should be taken not at the midpoint of the sample interval but midway between the summary points. At this abscissa, the slope of the linear and the quadratic forms coincide so that at this point the slopes of both the linear trend and the curvature are summarized.

In past application, the choice of intervals has been largely arbitrary; generally these successive subranges have been taken of equal length. In this paper, the power of the method is generalized so that the computer selects each subrange according to rules which take account of the density of data points and variations in local curvature. A useful decision procedure that may be new to the theory of smoothing is to calculate a subsidiary curve showing the variation of the uncertainty of the summary ordinates with number of data points in the first interval. An optimum selection can be made by a trade-off rule [7]. The algorithm then successively computes a series of summary value pairs, with unequal spacing, that provide a representation of the original time series. Noise in the observed values can be treated by the application of weights, chosen to yield stable and robust statistical estimates [8, 9].

The generalized process described here has been tested in a number of applications. It proves to be computationally straightforward and not unduly time consuming, if handled on an efficient program and computer.

2. Mathematical Formulation

Consider $n \geqslant 4$ points (x_i, y_i) of equal weight in an interval of the argument. Let the pair of summary points in the interval be (X_1, Y_1) and (X_2, Y_2). The linear leastsquares fit to the data points, passing through the summary points, is

$$y = \frac{Y_2(x - X_1)}{(X_2 - X_1)} + \frac{Y_1(X_2 - x)}{(X_2 - X_1)}. \tag{1}$$

The normal equations for the ordinates are

$$\begin{bmatrix} \sum \frac{(x_i - X_2)^2}{(X_2 - X_1)^2} & -\sum \frac{(x_i - X_1)(x_i - X_2)}{(X_2 - X_1)^2} \\ -\sum \frac{(x_i - X_2)(x_i - X_1)}{(X_2 - X_1)^2} & \sum \frac{(x_i - X_1)^2}{(X_2 - X_1)^2} \end{bmatrix} \begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix} = \begin{bmatrix} -\sum \frac{y_i(x_i - X_2)}{(X_2 - X_1)} \\ \sum \frac{y_i(x_i - X_1)}{(X_2 - X_1)} \end{bmatrix} \tag{2}$$

The quadratic least-squares fit to the data points, also passing through the summary points, is

$$y = \frac{Y_2(x - X_1)}{(X_2 - X_1)} - \frac{Y_1(x - X_2)}{X_2 - X_1} + A(x - X_1)(x - X_2). \tag{3}$$

The normal equations for the ordinates in this case are

$$\begin{bmatrix} \sum \frac{(x_i - X_2)^2}{(X_2 - X_1)^2} & -\sum \frac{(x_i - X_1)(x_i - X_2)}{(X_2 - X_1)^2} & -\sum \frac{(x_i - X_1)(x_i - X_2)^2}{(X_2 - X_1)} \\ -\sum \frac{(x_i - X_1)(x_i - X_2)}{(X_2 - X_1)^2} & \sum \frac{(x_i - X_1)^2}{(X_2 - X_1)^2} & \sum \frac{(x_i - X_1)^2 (x_i - X_2)}{(X_2 - X_1)} \\ -\sum \frac{(x_i - X_1)(x_i - X_2)^2}{(X_2 - X_1)} & \sum \frac{(x_i - X_1)^2 (x_i - X_2)}{(X_2 - X_1)} & \sum (x_i - X_1)^2 (x_i - X_2)^2 \end{bmatrix} \begin{bmatrix} Y_1 \\ Y_2 \\ A \end{bmatrix} = \begin{bmatrix} -\sum \frac{y_i(x_i - X_2)}{(X_2 - X_1)} \\ \sum \frac{y_i(x_i - X_1)}{(X_2 - X_1)} \\ \sum y_i(x_i - X_1)(x_i - X_2) \end{bmatrix}. \tag{4}$$

It follows immediately, when Eqs. (2) are substituted into the first two equations of (4), that

$$A\Sigma(x_i - X_1)(x_i - X_2)^2 = 0 \tag{5}$$

and

$$A\Sigma(x_i - X_1)^2(x_i - X_2) = 0, \tag{6}$$

from which X_1 and X_2 can be determined.

In particular, subtracting (5) and (6) yields

$$\Sigma(x_i - X_1)(x_i - X_2) = 0. \tag{7}$$

Let $\Sigma x_i = n\bar{x}$, $\xi = x - \bar{x}$, $\xi_1 = X_1 - \bar{x}$, $\xi_2 = X_2 - \bar{x}$; and put $\Sigma\xi^2 = n\mu_2$, $\Sigma\xi^3 = n\mu_3$, summed over n data points.

It then follows by substitution that ξ_1, ξ_2 are the roots of the quadratic

$$t^2 - (\mu_3/\mu_2)t - \mu_2 = 0. \tag{8}$$

Hence we can compute X_1 and X_2 and the corresponding ordinates follow by inverting the matrix (2).

More generally, each point is associated with a weight $w_i = \sigma^2/\sigma_i^2$, where σ^2 is the variance of a y_i sample value of unit weight. The weights can be introduced in appropriate places in the above equations. In the usual way, if we operate on (2) with the variance operator, we find

$$\text{var } Y_1 = \frac{(X_1 - X_2)^2\, \sigma^2}{\sum w_i(x_i - X_2)^2} \tag{9}$$

and

$$\text{var } Y_2 = \frac{(X_1 - X_2)^2\, \sigma^2}{\sum w_i(x_i - X_1)^2}\,. \tag{10}$$

Also, calculation yields $\text{cov}(Y_1, Y_2) = 0$, so that the summary points have the special property that the uncertainties of their ordinates are uncorrelated.

The summary gradient for the interval in question is, from (1),

$$dy/dx = (Y_2 - Y_1)/(X_2 - X_1) \tag{11}$$

and the corresponding abscissa is $x = (X_1 + X_2)/2$.

Because the covariance vanishes, the variance of the gradient is simply $(\text{var } Y_1 + \text{var } Y_2)/(X_2 - X_1)^2 = V^2/(X_2 - X_1)^2$ (say).

3. Description of the Numerical Procedure

Several programs were written to compute summary values using the above algorithms. For the essentials, consider a single version with options, called SUMMOOTH, for accomplishing solutions of (8) and (2). It includes an option for computing (8), (2), and the gradient (11).

Initially, let the first interval INT for the number of sample points be fixed such that $x_1 < x_i < x_{\text{INT}}$. The program then computes the pair of summary values for this range of x. By means of a program loop the first point at x_1 is then discarded and the next point at $x_{\text{INT}+1}$ is added; another pair of summary points is calculated for the new interval and so on. INT thus defines a sample window of fixed width which moves along the time series until the terminal point at x_n is reached. In this case, the summary pairs are at unequal values of the argument and, in general, overlap. They may be printed or plotted to provide a set of smoothed values to replace the original raw series x_i.

It was found that, for convenience in this computation mode, only a subset of smooth values need be printed or plotted. The rule adopted was to have the window move forward until the trailing summary value of the current pair had an abscissa equal to that of the point midway between the pair previously adopted. The resulting set of points representing the original time series usually represented satisfactorily the main fluctuations in the series but filtered out the highest frequencies (see, for example, Fig. 1).

At this stage, the smoothing is a function of INT which has been arbitrarily selected. In practice, several runs can be made for a sequence of values of INT and the appropriate set of smoothed values then selected (perhaps based upon the number of points needed or the size of the variances associated with the summary values). This subjectivity (i.e., arbitrariness in INT) can be removed in a number of ways. One procedure is to adopt a principle of symmetry and by repetitive computation with a sequence of values of INT select a value of INT such that the resulting sets of smoothed values are approximately equal (say in a least-squares sense) whether the window moves from the left (x_1, x_2,...) or the right (x_n, x_{n-1},...).

After numerical experimentation, another procedure was adopted as an option in SUMMOOTH as a selection rule. In this case, the principle of selection was based upon the simultaneous minimization of INT and the variance of the ordinates (9) and (10) or the gradient (11). In many cases, it was found that, at least for time series with variances σ^2 roughly stationary as a function of x_i, the longer the width of the interval summarized the smaller the average value of $(\text{var } Y_1 + \text{var } Y_2)/(X_2 - X_1)^2$. In other words, the trade-off curve between these quantities was roughly a rectangular hyperbola. The point on this curve nearest to the origin was selected automatically as defining the optimal summary interval width. An example of the use of this principle is give in Section 5.

Finally, an option was tested that provided for smoothing with a moving interval window of variable width. The computation of INT (x) was done by requiring that the variance of an observation be maintained constant for every pair of summary

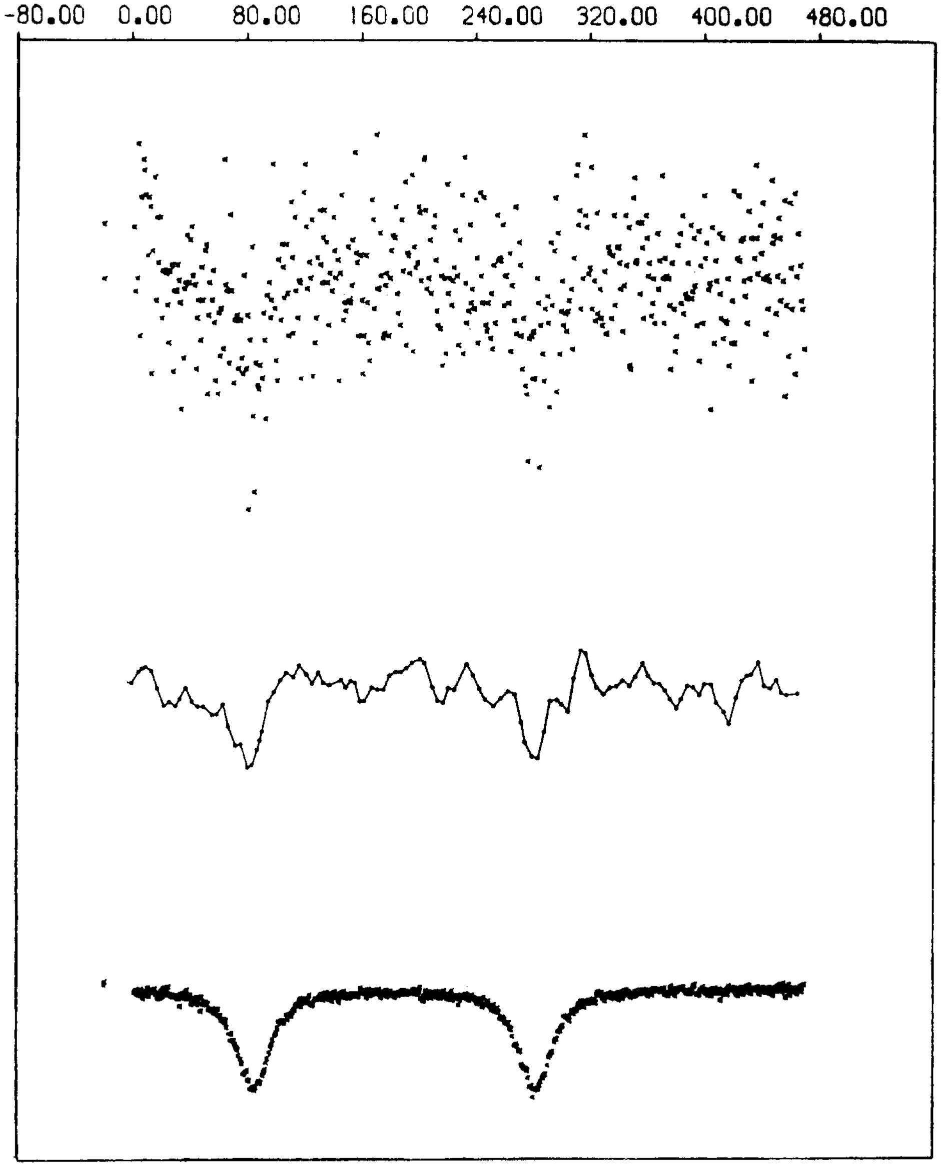

FIG. 1. Time series with unequal intervals for a Mosshauer spectra. The upper plot shows the raw data with large dispersion. The center plot shows the top data smoothed using the summary value method with a moving window of fixed width with 20 data points. The bottom plot is the experimental spectrum obtained with finer instrumental setting.

points. The programmed method proceeded by successive trials and was relatively time consuming. It does, however, help deal with the problem of variation in sampling density in the original time series.

The first test of SUMMOOTH was carried out on the same scarce and noisy data used by Talmi and Gilat [10]. The points are samples from a Mossbauer spectrum experiment. The aim of these authors was to show how well their smoothing algorithm, using special functions, filtered the noise and detected the true experimental features in such a case. In Fig. 1, results with the summary value method for just one set of the spectral data are displayed. At the top are the original noisy data; in the center is the smoothed variation using the simple unweighted version of the summary point algorithm. At the bottom is the spectrum published by Talmi and Gilat for a data sample measured with less dispersion. It is evident that the method of summary values has resolved the fine structure of the spectrum closely.

The details are as follows. The raw time series consisted of 460 widely scattered points at unequal values of the argument. A sequence of initial intervals was used (INT = 5, 8, 10, 15, 20) with SUMMOOTH to generate, from the unweighted data, tables of summary values. The case reproduced for comparison in Fig. 1 had INT = 20 and plotted points were selected by the bisection criterion described above. The points in Fig. 1 have been simply joined by straight lines. The method has successfully resolved the two spectral lines although some noise remains having various periodicities. Comparison with the three smoothed spectra for this data published by Talmi and Gilat shows that the smoothing achieved by the above simple application has produced a spectrum of about the same quality as their best case [10, Fig. 3, weight = 1]. The present method also tabulates the standard errors of the ordinates (not plotted) using (9) and (10).

4. Earthquake Prediction

In recent years it has been proposed that sometimes earthquakes are preceded by changes in the physical properties of the rock in the vicinity of the earthquake source [4]. These precursory changes cause the velocity of seismic waves to vary; in particular, the longitudinal P wave velocity v_p might decrease by up to 15 % in a period of months or years before moderate to large earthquakes.

The observational analysis is simply to plot the difference in time of arrival of S and P waves $(t_s - t_p)$ at a station from a source against the time of arrival of P (t_p). The slope of the curve (usually nearly linear) is $t_s/t_p - 1$, which gives at once t_s/t_p and hence v_p/v_s, the ratio of the apparent mean P to S velocity. In a region of concern, the stations and earthquake sources would usually be chosen so that the waves passed through the region. Because the occurrence of earthquakes is irregular, the resulting time series of v_p/v_s values is at unequal intervals of time. Further, because of difficulties in selection of corresponding P and S phases on the seismograms, and errors in the location of the sources, the resulting t_s/t_p (or v_p/v_s) values are subject to considerable errors of observation. Some rejection and weighting scheme is almost inevitable.

A typical display of the v_p/v_s time-series is graphed in Fig. 2a. The points are from individual earthquakes, which of course, do not occur at equal intervals of time. Such a time series might already be the result of a bandpass filter or rejection law. The sometimes crucial effect of this process is ignored here. The data used are based on various published time series of this type for earthquakes in California, Japan, and the USSR [11]. An overall interval of 4 years is used. The question then is: Are there any anomalous intervals defined by dips or bays in the v_p/v_s curves? If there are, a common prediction hypothesis states that (i) the time width of the bay is proportional to the magnitude of the impending earthquake, and (ii) the impending earthquake will occur shortly after the return of the v_p/v_s values to their normal range.

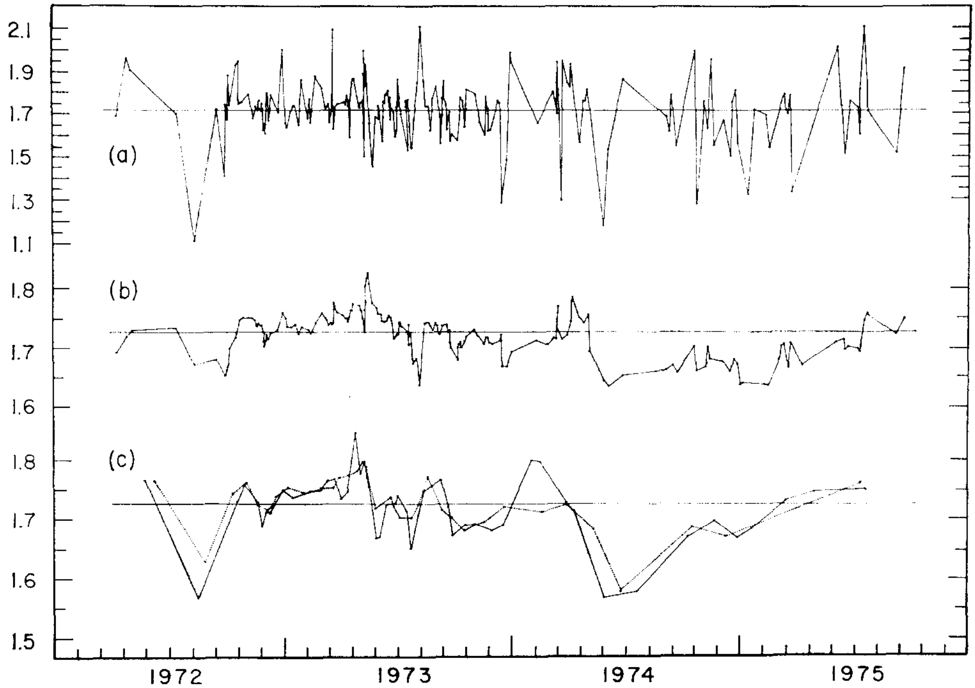

FIG. 2. A comparison of a time-series of v_p/v_s ratios for 4 years. Note that the ordinate scale changes between (a) and (b) and (c). Series (a) is the raw data with sparse and dense sections. Series (b) is the raw data after standard smoothing by a running mean. At the bottom (c) two smoothed series are shown using SUMMOOTH. The continuous line is from a window with 20 data points; the dotted line is from a window with 30 points.

First, consider the effect of smoothing the time series by a running mean. Let y_i be the ith raw value of v_p/v_s, and s_i be the corresponding smoothed value. The smoothing formula

$$S_i = A \sum_{k=0}^{\infty} (1 - A)^k \, y_{i-k} \tag{12}$$

is sometimes used. With $A = 0.1$, for example, the smoothed values are broad nonsymmetrical averages using moderately weighted adjacent values effectively extending out to 5 or 6 sequential positions.

The time series S_i, smoothed using (12), is drawn in Fig. 2b. It is clear that the unevenly spaced data have given rise to fluctuations of small amplitude in the smoothed curve. From a naive point of view, the bay of 12 months' duration beginning in early 1974 might be interpreted as significant. It is unclear, however, how to apply any objective significance test using the above methodology.

Let us now compare the above treatment with a smoothing using the summary value algorithm. We have 220 points (x_i, y_i) as shown in Figure 2a. Program SUMMOOTH was used to compute summary values for a sequence of values of INT. Resolution of the longer period fluctuations, similar to that obtained in Fig. 2b using (12), was found with INT = 20. Summary points selected by the midpoint method for this case are shown as a continuous line in Fig. 2c. For visualization only, the 50 summary points have been joined by straight line segments. The rather close resemblance of Figs. 2b and c is evident.

For comparison, the 38 points in Fig. 2c joined by dotted lines are every tenth pair of summary points calculated by SUMMOOTH with a moving window of width INT = 30. The effect of summarizing both the linear and parabolic trends over a wider interval can be clearly seen.

It is of interest in this case to examine explicitly the variances of the summary points from (9) and (10). The numerical values for INT = 20 are listed in Table I. The values of the standard errors given under the third column are calculated putting $w_i = 1$, all i. These values, of course, are not independent of each other as ordered in Table I. Only the variances of each pair of summary values located in the table at (X_1, X_3), (X_2, X_5), $X_4, X_7)$, etc., are uncorrelated. The largest s.e. is $Y_1 \pm 0.52$ and the smallest is $Y_{42} \pm 0.24$. A representative value is 0.30. It will be seen from the vertical scale in Fig. 2 that the fluctuations in the smoothed series are well within these bounds so that the significance of the remaining deviations is doubtful.

5. Summary Value Travel-Time Gradients

As an illustration of use of the algorithm to compute directly a set of summary gradients (derivatives) from a time series, numerical analysis was done using (11), on a table of published empirical seismological travel-time curves. The values used are from the 1968 Seismological Tables for P waves [12]. A travel-time y_i (seconds) is given for each distance, in angular degrees, x_i tabulated at 20° (1°) 104°.

It was in this context that Jeffreys first applied the method of summary values [3] but the present procedure is quite different. Jeffreys used the method (with consecutive adjacent intervals of fixed width) to obtain a smoothed set of summary travel times from the raw measurements. Because the resulting summary times were unequally spaced, he then interpolated them to equal intervals. Only then were the gradients $(\Delta y/\Delta x)$ found using divided differences. But (11) allows the optimal gradient to be

TABLE I

Smoothed v_p/v_s Series (Int = 20)

X_i	Y_i	SE
1972.39	1.76	.52
1972.62	1.57	.46
1972.79	1.72	.24
1972.81	1.81	.36
1972.82	1.75	.25
1972.88	1.72	.30
1972.90	1.68	.28
1972.91	1.71	.27
1972.93	1.70	.33
1972.98	1.74	.32
1973.03	1.73	.37
1973.10	1.74	.38
1973.15	1.74	.30
1973.19	1.76	.30
1973.21	1.76	.27
1973.25	1.73	.34
1973.27	1.74	.32
1973.31	1.84	.37
1973.33	1.77	.29
1973.35	1.79	.25
1973.36	1.76	.27
1973.40	1.66	.37
1973.42	1.66	.44
1973.44	1.72	.33
1973.47	1.72	.27
1973.48	1.72	.30
1973.49	1.73	.30
1973.52	1.71	.28
1973.54	1.64	.32
1973.57	1.70	.32
1973.60	1.74	.35
1973.64	1.75	.31
1973.68	1.76	.30
1973.71	1.71	.28
1973.73	1.66	.31
1973.79	1.68	.29
1973.83	1.68	.36
1973.90	1.67	.30
1973.96	1.68	.34
1974.07	1.79	.38
1974.16	1.79	.33
1974.23	1.72	.24
1974.26	1.71	.27
1974.41	1.56	.36
1974.54	1.57	.50
1974.76	1.66	.31
1974.87	1.69	.28
1974.98	1.66	.28
1975.05	1.67	.31
1975.19	1.72	.31

TABLE 2

Summary Gradients of the 1968 Travel-Time Curve

Distance (x_i)	Summary gradient ($\Delta y/\Delta x$)	Interpolated gradient
27.5	9.0752	8.9704
32.5	8.7713	8.7699
36.5	8.5357	8.5417
40.5	8.2631	8.2690
44.5	7.9904	7.9916
48.5	7.6992	7.6907
52.5	7.4042	7.4028
56.5	7.1071	7.1150
60.5	6.8364	6.8281
64.5	6.5677	6.5685
68.5	6.2890	6.2985
72.5	5.9815	5.9723
76.5	5.6746	5.6821
80.5	5.3650	5.3649
84.5	5.0359	5.0198
88.5	4.7833	4.7598
92.5	4.6372	4.6293
96.5	4.5713	4.5702

calculated for each summary interval without intervening interpolation. This method was used on the above tables with a sequence of values for INT using SUMMOOTH as before. The resulting summary gradients (giving each observation unit weight) are listed in Table II for INT = 10. The values differ in the second decimal place with the corresponding gradients given in column 3, calculated by differencing the P tables [12]. Because the gradients are used for determining the velocity in the Earth from numerical inversion of the Herglotz–Abel integral, small systematic errors in the gradient estimates may be important. Thus the present method would appear to offer advantages over the previous one.

Finally, in Fig. 3, the quantity V for the summary gradient, assuming unit variance for an observation of unit weight, is plotted for each value of INT adopted. (In this example, because the x_i are at equal intervals and each point has the same weight, the variance for every summary gradient is equal for a fixed INT.) As discussed in Section 3, the result is a trade-off curve that can be used to select a value for the interval width INT. The desirable corner position (for the units used here) corresponds to about INT = 9 and $V = 0.6$ (seconds). In this application of the trade-off curve, the ordinate can be thought of as proportional to the amount of smoothing and inversely proportional to the resolution of fine detail in the time series. It should be noticed that this use (like many others) of the trade-off algorithm is not dimension-free; a change in the scale of the abscissa (i.e. V) yields a different INT. If the trade-

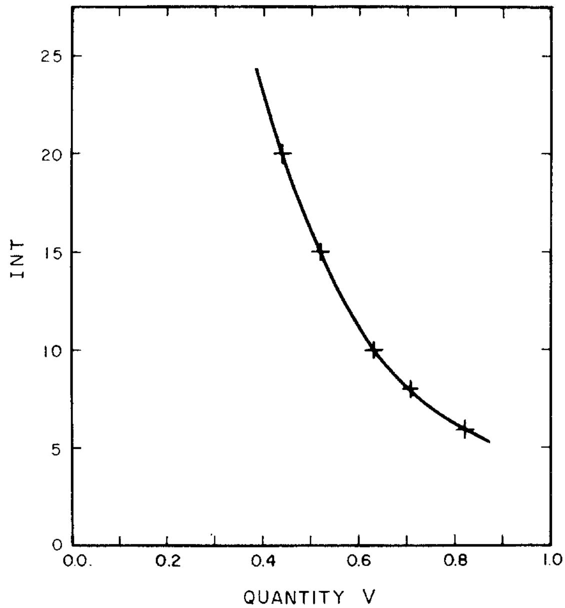

FIG. 3. A trade-off curve of the number of data points (INT) in the summary interval versus the quantity V. The computed 5 points are from the calculation of summary gradients of the unsmoothed 1968 seismological P times.

off curve is assumed to be a true rectangular hyperbola, then if V is always scaled to achieve the standard form of the rectangular hyperbola, a more objective rule is obtained.

6. Conclusion and Outlook

Availability of high-speed computers allows the generalization of a smoothing algorithm, called the method of summary values, devised by H. Jeffreys. Rather than subdividing, in a subjective way, the original time series into adjoining intervals and then summarizing the data in each cell by a pair of summary points, the present algorithm computes summary values for overlapping intervals according to prespecified selection rules or general principles.

Tests of a program that generates the smoothed values demonstrate the advantages and disadvantages of the new method. The time series need not be at equal intervals of the argument and variations in sample density may be automatically allowed for by a requirement on the constancy of the variances of the summary ordinates. When the width of the moving interval window is plotted against these variances, the resulting trade-off curve gives a rule for selection of the optimum resolution of periodicities in the time series.

An extension of the original derivation of the method of summary values gives a simple formula for the direct estimation of the summary gradient within the summary interval together with its variance. These formulas may find considerable application in the construction of revised seismological traveltime slowness and attenuation curves as well as the determination of seismic velocity distributions.

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