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FAST DIGITAL NOISE FILTER CAPABLE OF LOCATING SPECTRAL PEAKS AND SHOULDERS

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16. ABSTRACT

Experimental data frequently have a poor signal-to-noise ratio which one would like to enhance before analysis. With the data in digital form, this may be accomplished by means of a digital filter. A fast digital filter based upon the principle of least squares and using the techniques of convoluting integers is described. In addition to smoothing, this filter also is capable of accurately and simultaneously locating spectral peaks and shoulders. This technique has been adapted into a computer subroutine, and results of several test cases are shown, including mass spectral data and data from a proportional counter for the High Energy Astronomy Observatory.

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TABLE OF CONTENTS

LIST OF ILLUSTRATIONS

TECHNICAL MEMORANDUM X-64707

FAST DIGITAL NOISE FILTER CAPABLE OF LOCATING SPECTRAL PEAKS AND SHOULDERS

INTRODUCTION

Much valuable information from an experiment may be lost because of a poor signal-to-noise ratio. The source of this unwanted noise is usually a combination of ground loops, transient currents, reading errors, using equipment near the limits of its range, etc. In most experiments, one can assume that the noise is a random event distributed normally about the true signal. This is a Gaussian-shaped distribution, with most of the deviations caused by noise occurring within one standard deviation of the signal. It is normally assumed that the standard deviation of the noise is independent of the signal value and is also constant throughout the experiment.

Under such assumptions, it is possible to utilize several techniques for enhancing the signal-to-noise ratio. An example is the simple RC filter used to remove the high-frequency noise component from an analog signal. In recent years, however, more and more experimentalists have turned to computers for analyzing results, and somewhere in the course of the experiment it is necessary to digitize the stream of analog data. Unfortunately, the noise present in the analog signal carries over into the digital signal.

Thus, the need arises for a digital filter which is capable of enhancing the digitized signal. Several of these filters exist [1-4], and this report will describe one based upon the principle of least squares. The idea behind this filter was presented by Savitsky and Golay [5] and has been expanded and programmed by the authors to handle spectral data. This type filter has been found advantageous because of its high speed and because it not only "smooths" the data, but simultaneously finds the peaks and shoulders present in the spectrum. The following sections will describe the principles of the filter and its implementation in spectral analysis.

THE THEORY OF CONVOLUTING INTEGERS

The object of this digital filter is to remove as much noise as possible without degrading the signal. The filter operates by modifying a given point to be some function of itself and nearby points. An RC filter can use only past information, and this introduces a unidirectional distortion into the data; i.e., phase shift. A digital filter, however, can take advantage of the stored array of data to utilize both past and future points, thus providing a better smooth than an analog filter.

Two assumptions concerning the data must be met if the filter is to be effective: (1) the data must occur at equally spaced intervals along the abscissa, and (2) the curve formed by the data in the filter must be reasonably smooth [5]. The first of these assumptions is always met in computer work because the abscissa is actually the time interval at which the data are sampled, and this is equal interval and stable to 0.01-percent accuracy or better. This report will deal primarily with the filtering of the intensity since it is the signal of main interest.

A simple digital filter is a moving weighted average. The j^{th} point modified by the $2m+1$ points of which it is the center:

$$y_j^* = \sum_{i=-m}^{m} c_i y_{j+i} / N \quad . \tag{1}$$

The coefficients c_i are integers which are chosen to give the desired weighting, and N is the normalization factor (in this case, N is equal to $2m+1$). By allowing j to run through the index of the array, the data are smoothed using only simple arithmetic operations. It is clear that m can be set to any value, giving a $2m+1$ point filter.

The c_i coefficients are called convoluting integers for the following reason. The filter can be considered an operator which forms the smoothed data $y^*(t)$ by integrating the raw data $y(t)$ with a weighting function $w(t)$. Since the weighting at a point depends upon the time difference between the weighted point and the point being smoothed, the filtering operation can be written [6]

$$y^*(t) = \int w(\tau)\, y(t-\tau)\, d\tau \quad . \tag{2}$$

This integral is defined as the convolution of $y(t)$ with $w(t)$. In a digital filter the weighting function is of the form

$$w(\tau) = \sum_{i=-m}^{m} c_i\, \delta(\tau + i)/N \tag{3}$$

where $\delta(t)$ is the Dirac-delta function representing the discrete sampling of the data. Using this in equation (2) at time $t = j$ gives

$$\begin{aligned} y^*(j) &= \int \left[\sum_{i=-m}^{m} c_i\, \delta(\tau + i)/N \right] y(j-\tau)\, d\tau \\ &= \sum_{i=-m}^{m} c_i y(j+i)/N \quad . \end{aligned} \tag{4}$$

By equating $y(j+i)$ with y_{j+i}, this is seen to be identical to equation (1). Thus, the c_i's are known as convoluting integers.

While the moving weighted average works well for a quasi-dc signal, it tends to drastically distort a curve of large curvature, such as a peak. Thus, one would like to retain the simplicity of equation (1) but find a set of convoluting integers which does not alter the shape of the data. The most commonly used method for smoothly fitting a curve to a group of data points is the method of least squares; therefore; we are led to try fitting an n^{th} degree polynomial to $2\,m+1$ points such that the sum of the squares of the residuals is minimized. Our goal is to express the polynomial value at the center point in terms of the $2\,m+1$ unsmoothed points, and we will then regard this as the smoothed value of the center point. This method will be seen to provide not only a set of convoluting integers for smoothing, but also sets for finding the first n derivatives.

The problem is to fit a polynomial to $2m+1$ points and then replace the center point by its polynomial, or smoothed, value. Since the data points are assumed to be uniformly spaced and odd in number, they can be normalized and centralized to be integer values centered at zero [7]; i.e., $t_i = i$. The n^{th} degree polynomial is then of the form

$$f_i = \sum_{k=0}^{n} b_k i^k = b_o + b_1 i + \dots + b_n i^n \quad . \tag{5}$$

But we only require the value at $i = 0$, so clearly $y^* = f_o = b_o$. We find that the smoothed value at a point is merely the first coefficient of the best-fit polynomial centered at the point. By further taking derivatives of the polynomial, one can show

$$y^* = f_o = b_o$$

$$\frac{dy^*}{dt} = \frac{dy^*}{di}\frac{di}{dt} = \frac{1}{\Delta t}\frac{df_o}{di} = \frac{b_1}{\Delta t} \tag{6}$$

$$\vdots$$

$$\frac{d^s y^*}{dt^s} = \frac{d^s y^*}{di^s}\left(\frac{di}{dt}\right)^s = \frac{1}{(\Delta t)^s}\frac{d^s f_o}{di^s} = \frac{s!\, b_s}{(\Delta t)^s}$$

where Δt is the constant step size between abscissa points; i.e., the analog-to-digital conversion time. Thus, the smoothed value at the first n derivatives at the center point can be found by solving for the proper regression coefficients.

The solution for the regression coefficients b_s can be found in numerous texts on regression analysis and will not be given here. One can show that the solution is of the form

$$s!\,b_s = \sum_{i=-m}^{m} c_i y_i / N \quad . \tag{7}$$

This is identical to equation (1), with $j = 0$, since the points here are centralized. Thus, each b_s and, hence, each derivative can be evaluated by a set of c_i of convoluting integers. These integers depend on the order of derivatives (0 to n), the number of points (2 m+1), and the order of the polynomial ($n < 2\,m+1$). Large tables of these convoluting integers with their corresponding normalization factors can be found in Reference 5.

It is also possible to convolve two of these sets of integers together, resulting in a single set of integers which performs the operations of the two original filters simultaneously. This is decidedly advantageous for programming. Thus, if we convolve a 2 m+1 point n^{th} order smooth with a 2 p+1 point k^{th} order s^{th} derivative, we obtain

$$\frac{d^s y_o^*}{dt^s} = \frac{1}{N_s (\Delta t)^s} \sum_{i=-p}^{p} c_{i,s} \left(\frac{1}{N_o} \sum_{j=-m}^{m} c_{j,o}\, y_{i+j} \right)$$

$$= \frac{1}{N_o N_s (\Delta t)^s} \sum_{i=-p}^{p} \sum_{j=-m}^{m} c_{i,s}\, c_{j,o}\, y_{i+j} \tag{8}$$

$$= \frac{1}{N} \sum_{h=-(m+p)}^{m+p} d_h\, y_h$$

$$d_h = \sum_{\substack{i,j \\ i+j=h}} c_{i,s} c_{j,o}$$

where

$$N = N_o N_s (\Delta t)^s \quad .$$

The $c_{i,s}$ are the convoluting integers of the k^{th}-order derivatives, the $c_{j,o}$ are those of the n^{th} order smooth, and the d_h are those for the combined operation. The resulting filter has $2(m+p)+1$ points.

APPLICATION TO SPECTRAL ANALYSIS

This technique is easily adapted to a program which smooths data and also finds peaks and shoulders. The resulting filter can accept roughly 2500 points per second on a computer such as the Univac 1108. Figure 1 is a flow chart of the filter, and this section will discuss the various operations.

In addition to smoothing spectral data, one wishes to know the locations and intensities of the spectral peaks. When a small peak occurs very close to a larger peak, the smaller one appears not as a separate peak but as a shoulder; i.e., an unresolved peak. The problem of determining if shoulders are present and, if so, their precise location is a difficult task. However, utilization of the above approach has resulted in an accurate algorithm for finding peaks and shoulders.

These operations have been included by the authors in the form of a computer subroutine. Input arguments are the x and y data points and a cutoff level (usually ~ 0.1 percent of the maximum y) below which peaks are not considered. The smoothed data and the locations and intensities of all peaks and shoulders are returned to the main program. A description of the flowchart is given in the following paragraphs.

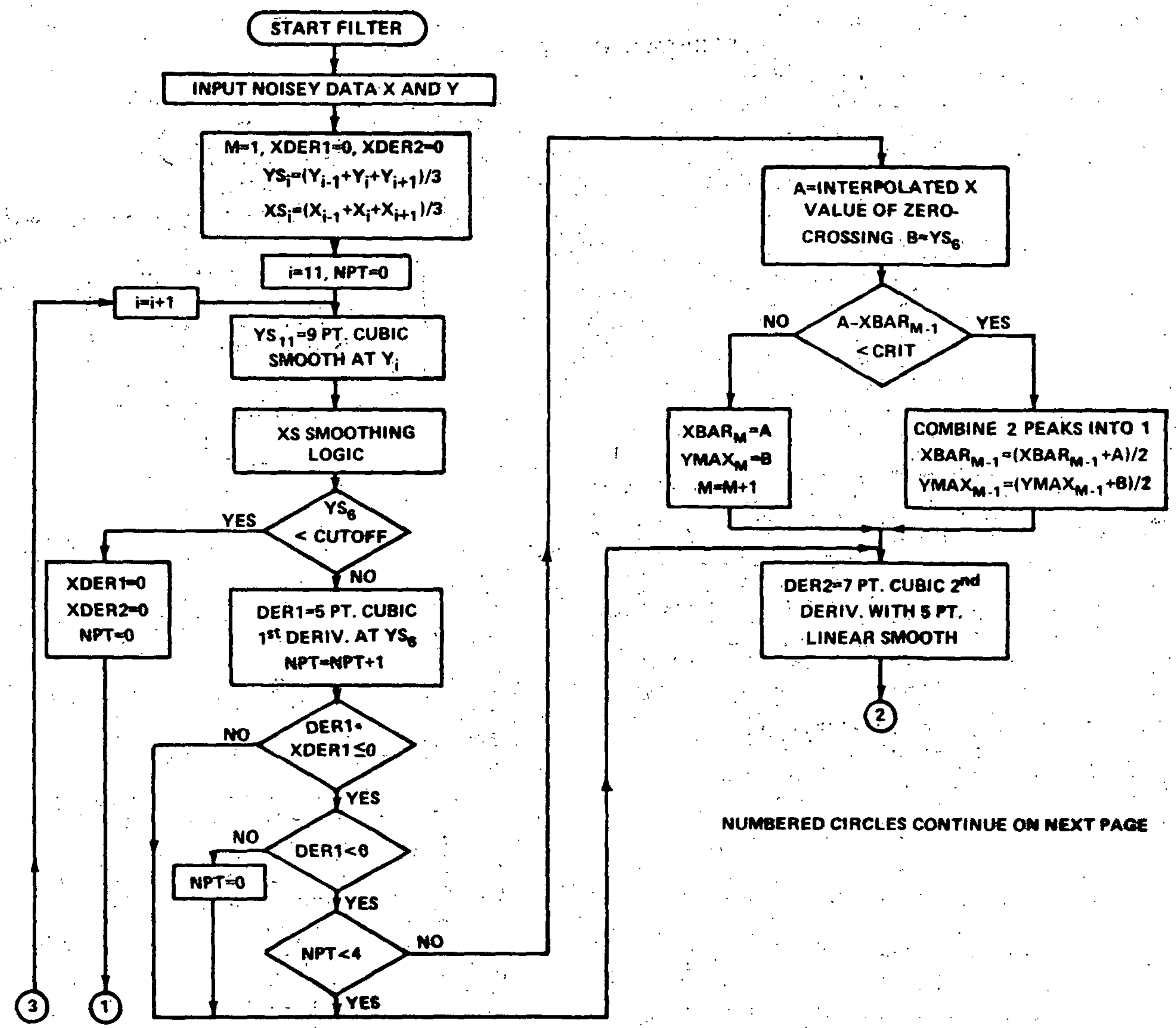
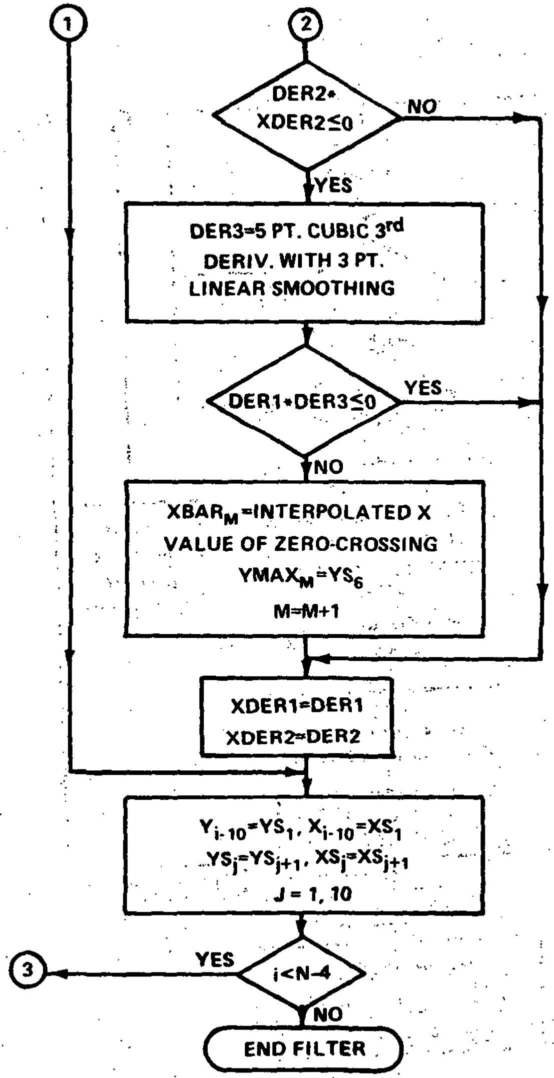


Figure 1. Digital filter flowchart.



PROGRAMMING SYMBOLS

X - ABSCISSA ARRAY
Y - INTENSITY ARRAY
N - TOTAL NUMBER OF POINTS IN X AND Y
YS - TEMPORARY ARRAY OF SMOOTHED INTENSITY VALUES
XBAR - PEAK LOCATION ARRAY
YMAX - PEAK HEIGHT ARRAY
M - TOTAL NUMBER OF PEAKS
DER1, DER2, DER3 – 1st 2nd AND 3RD DERIVATIVES AT YS_6
XDER1, XDER2 - 1ST AND 2ND DERIVATIVES AT YS_5
NPT – NUMBER OF POINTS PEAK HAS BEEN RISING
CRIT – CRITERION FOR COMBINING PEAKS

Figure 1. (Concluded)

Smoothing

A temporary 11-point array YS of smoothed points is used to ensure that only raw data are in the smoothing filter while only smoothed data are in the derivative filters. To get the filter started, the first 10 points of YS are initialized with a 3-point linear average of the corresponding points of Y. The main program loop does a 9-point cubic smooth of Y_i and stores it in the 11th point of YS:

$$YS_{11} = \left(-21\,Y_{i-4} + 14\,Y_{i-3} + 39\,Y_{i-2} + 54\,Y_{i-1} + 59\,Y_i + 54\,Y_{i+1} + 39\,Y_{i+2} + 14\,Y_{i+3} - 21\,Y_{i+4}\right)\Big/231 \quad (9)$$

Note the symmetry of the coefficients about Y_i, weighting past and future data equally. If YS_6, the center point YS array, is now greater than the cutoff level, the YS array proceeds to the next section. If not, then YS_1 is dropped off as a smoothed point and stored in place of the corresponding value of Y, transforming the raw data vector into a smoothed vector. The filter then moves forward a point by shifting YS_i to YS_{i-1} and calculating a new value of YS_{11} at the next point of Y.

Peak Finding

To use only smoothed data in the calculations, all derivatives are found at YS_6, the center of the YS array. The first derivative, DER1, is found with a 5-point cubic fit:

$$DER1 = YS_4 - 8\,YS_5 + 8\,YS_7 - YS_8 \quad . \quad (10)$$

The normalization factor is not used since absolute magnitudes are not needed for finding peak locations. This is because a peak is a relative maximum of the intensity, and, thus, occurs at a zero crossing; i.e., where the first derivative changes sign. To distinguish peaks from valleys, one must also require the change to be from positive to negative. Thus, if DER1 and its product with the derivative at the last point are negative, a peak has occurred between the points and may be located by linear interpolation. To prevent any remaining noise from appearing as a peak, the program requires the intensity to have risen for at least four consecutive points preceding a peak. Even the smallest of true peaks should easily exceed this if the digital convertor sampling rate is adequate for the analog frequencies in question. Following the check for a peak, the YS array moves to the next section.

Shoulder Finding

The second derivative is now found at the same point as the first derivative. Since the taking of higher-order derivatives greatly enhances the noise level, compensation is obtained by further convolving the derivatives with a linear smooth. Thus, to find the second derivative, DER2, a 5-point linear smooth is combined with a 7-point cubic second derivative:

$$\begin{aligned} DER2 = {} & 5\,YS_1 + 5\,YS_2 + 2\,YS_3 - 2\,YS_4 - 5\,YS_5 - 10\,YS_6 \\ & - 5\,YS_7 - 2\,YS_8 + 2\,YS_9 + 5\,YS_{10} + 5\,YS_{11} \,. \end{aligned} \tag{11}$$

This has the effect of smoothing the data twice without altering the output YS of smoothed data. A shoulder represents a zero crossing in the second derivative, which can be distinguished from other inflection points because the product of the first and third derivatives is positive at shoulders and negative at other zero crossings. Thus, the second derivative is checked for zero crossings in a manner similar to that used for finding peaks, and, if one is found, a 5-point cubic third derivative combined with a 3-point linear smooth is calculated:

$$DER3 = -YS_3 + YS_4 + YS_5 - YS_7 - YS_8 + YS_9 \,. \tag{12}$$

The product of equation (12) with the first derivative then determines whether a shoulder has been found. The intensity at this point is misleading because of the influence of the larger peak nearby. Practice has shown that 90 percent of the intensity is a reasonable guess as to the true peak height. With exceptionally poor data, even the doubly convoluted smoothing is often not enough to offset the sensitiveness of the shoulder finder, and erroneous shoulders may be located. To overcome this, it may be necessary to expand the number of points in the filter and perform an additional linear smooth before finding the second derivative.

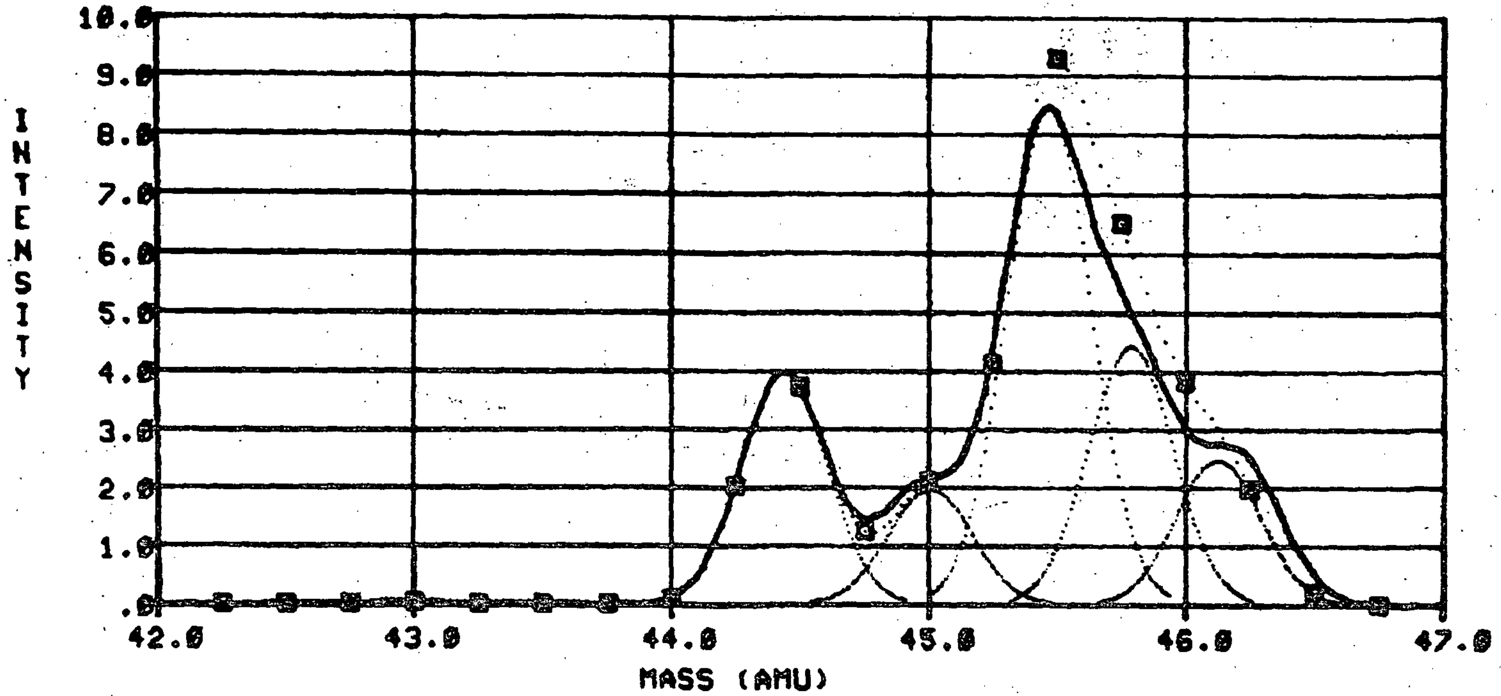
Following the finding of a peak, a pre-set criterion is used to determine if the peak is reasonably distant from the preceding peak or if it is so close that they should be combined into one peak. In case of shoulders, the location and intensity are generally in error from the true values by a few percent. This can be corrected by the use of an additional subroutine which performs multiparameter optimization. The authors are presently preparing a note on this subject. Having completed these operations, YS_1 is dropped as a smoothed point, the array is shifted forward a point, and the loop is started over by calculating a new YS_{11}.

TEST CASE RESULTS

Figure 2 shows the results of filtering a mass spectrum from a residual gas analyzer, the authors' main application of the subroutine. The spectrum in this case is synthetic, made by combining Gaussian peaks with the locations and intensities listed in the figure as Input. The values determined by the filter are listed under Zero Crossing. The peaks range from intensities of 0.04 (not even visible) to 8.0, a factor of 200. To make the spectrum more realistic, Gaussian-distributed random noise with a standard deviation of 0.01 was added.

Had the mass spectrum been real, it would have been necessary to smooth the mass values. An 11-point linear smooth operates well for a quadrupole spectrometer with a linear sweep. For a cycloid spectrometer, swept by an RC decay, a linear smooth of the logarithms of the mass values followed by exponentiating the result gives satisfactory values. However, for the synthetic spectrum, the mass values are generated accurately and require no smoothing. Thus, only the intensity values, generated at 40 points per AMU, were passed through the filter.

As Figure 2 will show, the filter correctly located the three peaks and three shoulders that were present. The curve passing through the black squares is the linear recombination of Gaussian waveforms using the determined values of the peaks. It follows the signal quite well except between 45.6 and 46.0. The problem here is that the peaks are so close that they overlap considerably, causing the signal at the 45.5 peak to be greater than



	SPECTRAL POSITION		SPECTRAL INTENSITY	
PEAK	INPUT	ZERO-CROSSING	INPUT	ZERO-CROSSING
1	43.000	42.964	.040	.041
2	44.440	44.441	4.000	3.996
3	44.975	45.010	2.000	1.983
4	45.450	45.472	8.000	8.490
5	45.800	45.790	4.000	4.450
6	46.210	46.130	2.500	2.482

INPUT
DE-CONVOLUTED
LINEAR SUM

Figure 2. Subroutine SM09 determination of peaks' and shoulders' synthetic spectrum.

the true peak height. Also, at the 45.8 peak (which, incidentally, would probably not even be found by eye), the estimation of 90 percent of the signal for the peak height was in error by 10 percent. The other four peaks are quite accurate, with an average mass error of 0.03 AMU and an average intensity error of 0.01.

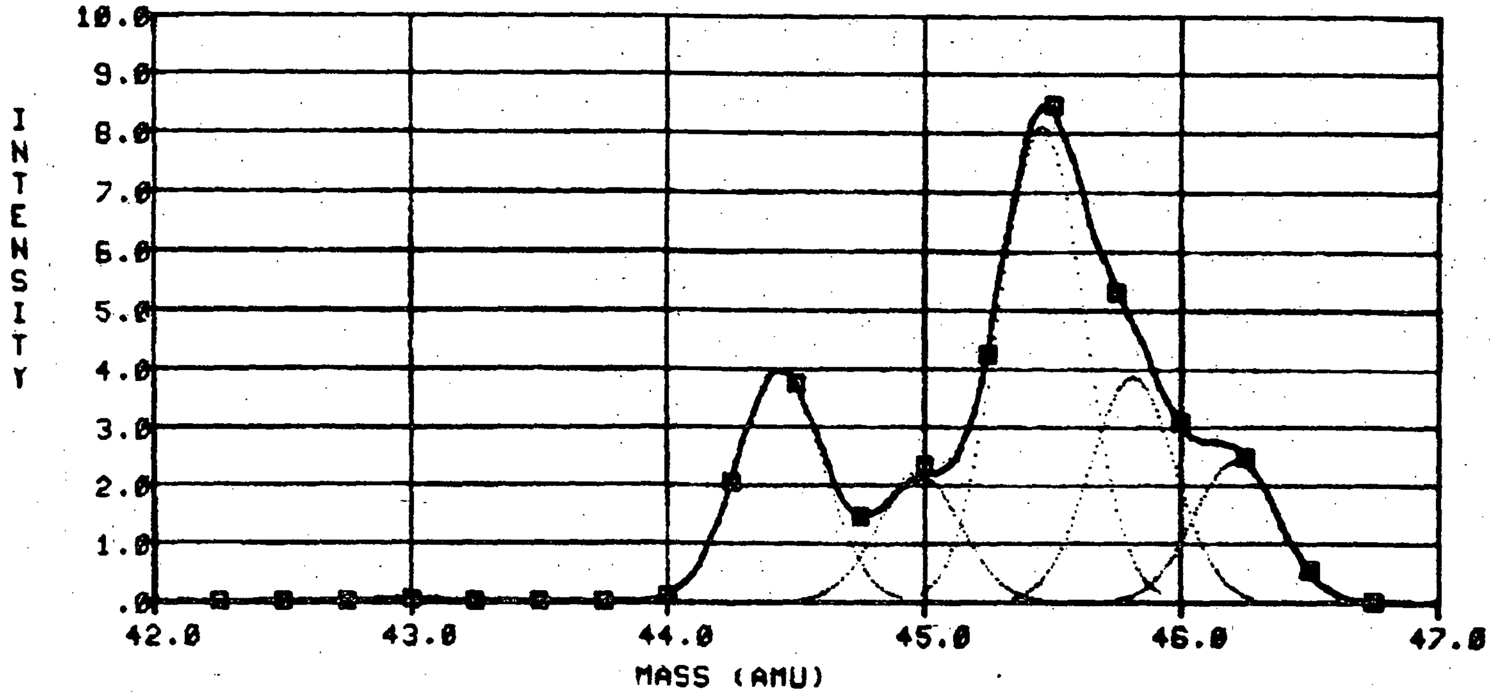
Figure 3 shows the result of passing the smoothed synthetic spectrum through a subroutine which performs multiparameter optimization. The positions and intensities of the peaks and shoulders found by digital filters are used as initial parameters in the optimization. An iterative technique then modifies these parameters so that the rms deviation between the smoothed and the optimized signals is minimum. As the figure shows, the combination of the filter with an optimization algorithm results in extremely accurate values of the parameters.

Figures 4 and 5 show the results of filtering data from a cosmic ray proportional counter associated with the High Energy Astronomy Observatory experiment and represent a good example of applying the filter to actual experimental results. The curve on the left of each figure is the raw data, and the one on the right is smoothed, optimized data. The curves, recorded on a multi-channel analyzer, were produced by radioactive decay of Fe-55. The right peak is the photo peak resulting from ion-pair production in the argon of the detector by 5.9 KeV photons produced by K-capture in the source. There is also a probability, although considerably less, that the same photons will remove a K electron from the argon, causing the so-called escape peak on the left. The presence of the two peaks is clearly seen in Figures 4 and 5. The YMAX and XBAR columns are the peak intensities and locations after using optimization subroutine. Note the success of the filter in removing excessive noise.

CONCLUSION

Based on these and other results, the authors feel that this digital filter, founded on the concept of convolving integers, is a reliable technique. In addition to its fast-smoothing capability, it also possesses the ability to easily and quickly determine derivatives and, hence, find peaks and shoulders. This should prove to be of value in many forms of spectroscopy.

It should be mentioned that the particular sets of convoluting integers used in the examples are not rigidly determined. They were chosen through



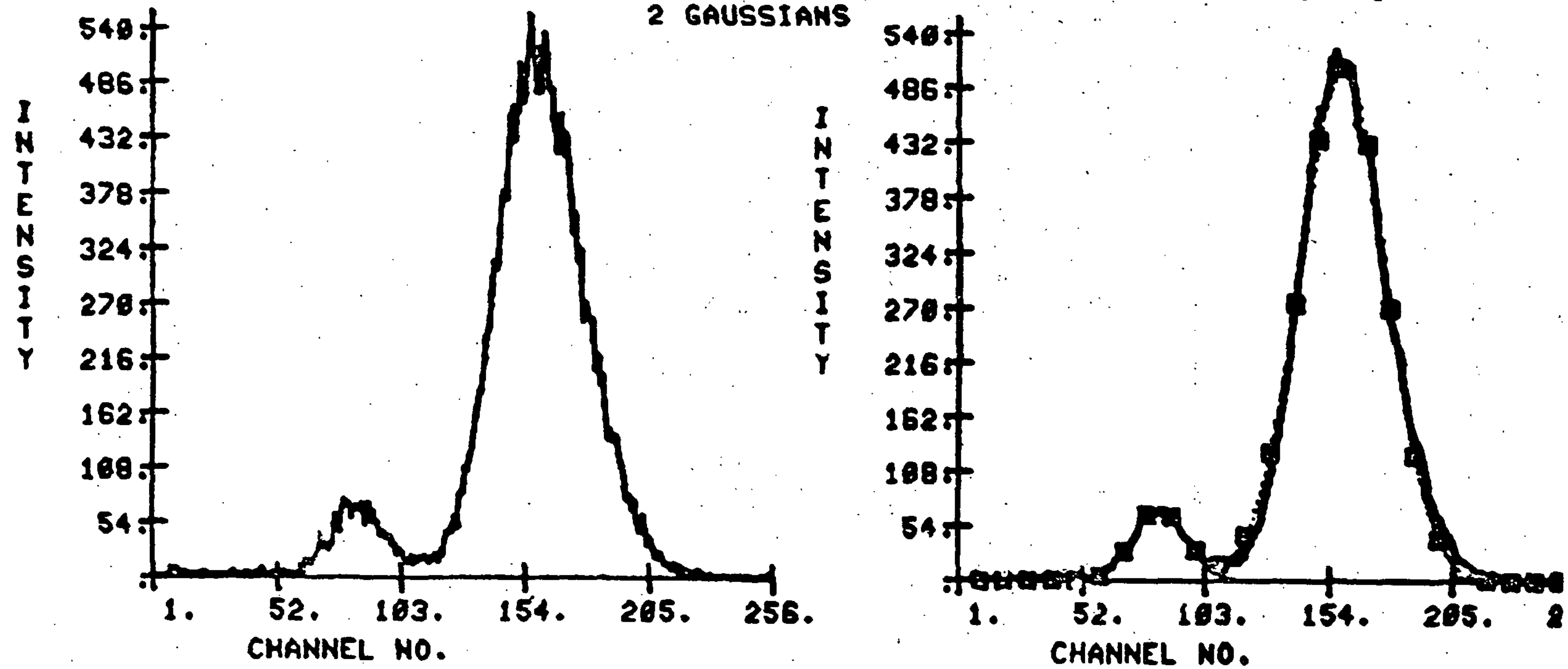
PEAK	SPECTRAL POSITION INPUT	SPECTRAL POSITION OPTIMIZED	SPECTRAL INTENSITY INPUT	SPECTRAL INTENSITY OPTIMIZED
1	43.000	42.997	.040	.040
2	44.440	44.440	4.000	4.004
3	44.975	44.985	2.000	2.169
4	45.450	45.457	8.000	8.116
5	45.800	45.814	4.000	3.888
6	46.210	46.218	2.500	2.430

INPUT
DE-CONVOLUTED
LINEAR SUM

Figure 3. Subroutine SM09 optimization of peaks' and shoulders' synthetic spectrum.

I. D.	TIME (MIN)	PRESSURE (TORR)	H. V. (VOLTS)	COLLIMATOR (MM)	DATE
1.B.	10	823.60	2000	.813	12/17/71

2 GAUSSIANS



YMAX	XBAR	BETA	FWHM	SIGMA	$SIGMA^2$
.70136E+02	.84787E+02	.28563E+02	.26416E+02	.11218E+02	.12584E+03
.49627E+03	.15985E+03	.39281E+02	.92469E+02	.18035E+02	.32526E+03

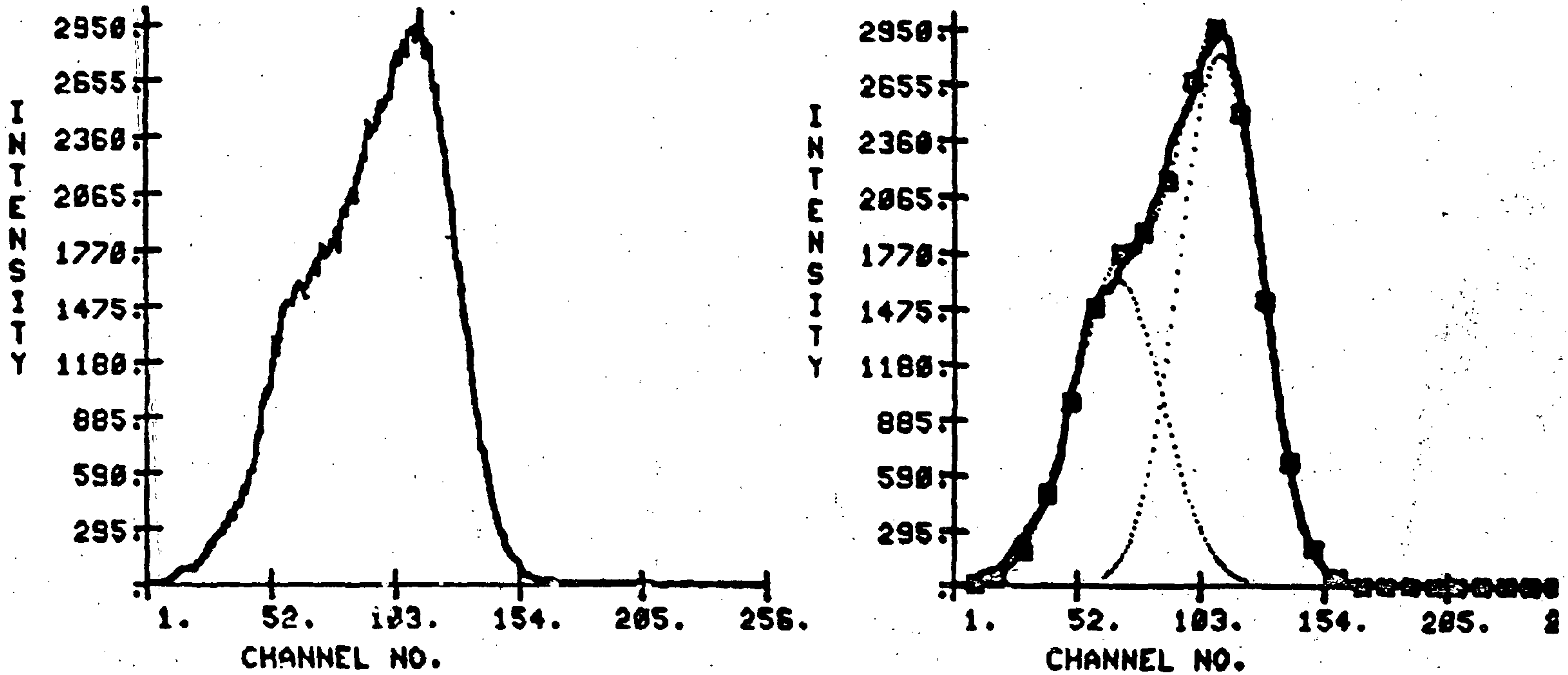
B	C	RESOLUTION KEV	RESOLUTION %	ABSCISSA RATIO R2	ABSCISSA RATIO R3
.75067E+02	.00000E+00	.17086E+01	.28572E+02	.46960E+00	.00000E+00

INITIAL RMS= .49571E+02 FINAL RMS= .10353E+02 TOTAL COUNTS .24852E+05

Figure 4. Proportional counter data.

I. D.	TIME (MIN)	PRESSURE (TORR)	H. V. (VOLTS)	COLLIMATOR (MM)	DATE
G R 14	2	746.89	1370	3.251	2/26/72

2 GAUSSIANS



YMAX	XBAR	BETA	FWHM	SIGMA	SIGMA^2
.15907E+04	.68996E+02	.67422E+01	.44245E+02	.18789E+02	.35303E+03
.27396E+04	.11121E+03	.21672E+02	.39778E+02	.16892E+02	.28534E+03
B	C	RESOLUTION KEV	RESOLUTION %	ABSCISSA RATIO R2	ABSCISSA RATIO R3
.42215E+02	.00000E+00	.28457E+01	.47586E+02	.37959E+00	.00000E+00
INITIAL RMS=	.52853E+03	FINAL RMS=	.45057E+02	TOTAL COUNTS	.19357E+08

Figure 5. Proportional counter data.

experience because they appeared to work the best. Each individual experiment should try different combinations of the number of points and the order of the polynomial to decide which works best for the type of data involved. As would be expected, increasing the number of points or decreasing the polynomial order causes less "bending" in the fit and, hence, better smoothing, but when carried too far, it distorts the signal shape. The necessary compromise must be determined on the basis of its merits in each individual experiment.

Further efforts are being made to use this technique in conjunction with Fast Fourier Transforms and other methods of data handling. Furthermore, the use of this filter in combination with optimization techniques results in extremely accurate spectral values in which the effects of noise have been almost entirely eliminated.

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APPROVAL

FAST DIGITAL NOISE FILTER CAPABLE OF LOCATING SPECTRAL PEAKS AND SHOULDERS

By T. R. Edwards and R. D. Knight

The information in this report has been reviewed for security classification. Review of any information concerning Department of Defense or Atomic Energy Commission programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.

This document has also been reviewed and approved for technical accuracy.

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