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GSSLRN-I

AN AUTOMATED LEAST-SQUARES
COMPUTER CODE FOR THE ANALYSIS
OF PHOTOPEAK SPECTRA

November 1969

AEC RESEARCH &
DEVELOPMENT REPORT

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GSSLRN-I

AN AUTOMATED LEAST-SQUARES COMPUTER CODE
FOR THE ANALYSIS OF PHOTOPEAK SPECTRA

By

G. D. Seybold

ANALYTICAL PHYSICS SECTION
REACTOR PHYSICS DEPARTMENT

November 1969

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ABSTRACT

A computer code, GSSLRN-I, is presented which is utilized for evaluations and statistical determination of photopeaks in photon spectra. The code performs evaluations of photopeak spectra using as input the digitized pulse height distribution which is output from a large multichannel analyzer. Photopeaks are located, functions are fit to each real peak, and the relative intensity of each fitted peak above the background continuum is calculated. The code contains various execution options and allows the user to obtain automatic and detailed plotting of the data and the results of each fit. The code is easily adaptable for analysis of any spectra which can be adequately defined by peaks represented in analytic form. Thus, it should be useful for application in such areas as; radiochemical analysis, analysis of reactor fuel burnup, half-life determinations, geological evaluations with respect to mineral content or time periods, analysis of Mbssbauer spectra and determination of elements in blood or body tissue,

TABLE OF CONTENTS

	<u>Page</u>
LIST OF FIGURES AND TABLES	v
I. INTRODUCTION	1
II. CODE REQUIREMENTS	2
III. SELECTION OF TECHNIQUES.	3
A. Peak Search Subprogram	3
B. Peak Fitting Subprograms	4
IV. ANALYTIC MODEL	6
A. GSSLRN-IA.	6
B. GSSLRN-IB	9
V. CODE DESCRIPTION	10
A. SEGMENT 1 (Input and Peak Search Routines)	13
B. SEGMENT 2 (Input Parameters and Peak Grouping Routines).	13
C. SEGMENT 3 (Fitting and Recycling Routines)	15
D. SEGMENT 4 (Calcomp Plotting Routines)	18
E. SEGMENT 5 (On-Line Plotting Routines)	19
F. Output Quantities.	21
G. Relative Differences Between GSSLRN-I A and GSSLRN-I B	21
VI. CONCLUSIONS.	22
VII INPUT REQUIREMENTS	25
Optional Input	30
Special Features.	31
VIII ACKNOWLEDGMENTS	
IX REFERENCES	34
APPENDIX A - PROGRAM EXECUTION	A-1
APPENDIX B - SAMPLE PROBLEM	B-1
DISTRIBUTION	D-1

LIST OF FIGURES AND TABLES

		<u>Page</u>
Figure 1	Pictures showing differences of first versus second order fitting.	5
Figure 2	Graph of test spectrum used.. . . .	8
Figure 3	Block diagram of GSSLRN-I.	11
Figures 4,5	Pictures of resolved multiplets from the test spectrum used with the program.	23
Table 1	Comparison of fitted results from GSSLRN-I A and GSSLRN-I B.	22

I. INTRODUCTION

The problem of analyzing high resolution photopeak spectra has been approached in various ways,^(1,2,3) However, each way uses a technique applicable to the problem which is unique, but all use a common approach which eliminates spectrum stripping,

One application of photopeak analyses is to the problem of determining total fuel burnup in nuclear reactors by gamma scanning for fission products. This specific problem is one which demands a good deal of accuracy. Research in this area is what initiated the development of GSSLRN-I.

The code is unique from other codes in that it utilizes fitting techniques which so far have not been used elsewhere for analyzing photopeak spectra. The code is based upon the least squares fitting techniques developed by Duane^(4,5) which are briefly second order Taylor's expansions with regression analysis. Varied tests have been incorporated into the code which rely on measurement variance, regression analysis and deviations from a least-squares fit in order to effectively resolve multiplets in complex photopeak spectra. The code is written in FORTRAN-IV for use on the UNIVAC-1108 computer,

Two stand-alone versions of the code, denoted as GSSLRN-I A, and GSSLRN-I B, exist. These codes differ in the manner in which the background of the spectrum is treated. More experience in spectrum analysis is needed to determine which of these treatments is the best and for that reason both are included in this report,

II. CODE REQUIREMENTS

The complexity of most gamma-ray spectra places some rather stringent requirements on the capabilities of a code which is to be used in a detailed and automated analysis of such spectra. The following is a list of some of the desired and/or required qualities of such a code,

- A peak searching algorithm which is reliable enough to be used on a routine basis,
- Second order fitting techniques which support multiple peak resolution when small intensity peaks are encountered under the wings of larger peaks,
- Validity of falsity determinations of each of the located peaks using statistical analyses. Since many photopeaks are contributing parts of multiplets, this condition is a difficult one to satisfy,
- Analytic function fits which adequately describe each valid photopeak such that the intensity of each peak can be evaluated with good precision. Also, in the case of partially resolved peaks, the areas under the curve for each peak must sum to the area under the function fitted to all the data,
- A consistently reliable measurement variance should be obtained which indicates the goodness-of-fit, and also provides a sound basis for suggesting the presence of hidden photopeaks,
- Input requirements should be designed such that the code is versatile and easy to use.
- Print-out options should be sufficiently flexible to provide virtually any desired level of detailed information (i.e., statistical information quantities, parameters for best fit, and plots),

III. SELECTION OF TECHNIQUES

If a computer code is to automatically analyze a set of data containing a complex spectrum of photopeaks, it must first scan the data set to locate all of the peaks present and then perform the fitting and evaluation necessary for analysis. These two processes, finding and fitting, are the heart of the code, GSSLRN-I, and are discussed in the following sections.

A, Peak Search Subprogram

Selection of a peak searching program was a necessity. A literature search was made to review the various approaches which had been used for this function. At the time of this review only a few techniques had been successfully demonstrated. The method chosen for GSSLRN-I was a technique used in program PALMUD as described by M. Mariscotti,⁽¹⁾ which utilizes second difference approximations with a variable choice of smoothes being applied to the counted interval of data in order to locate peaks. The original program⁽¹⁾ has been slightly modified to permit the user to optimize the method of search for his particular photopeak spectra. This optimization involves finding the set of input parameters which give the best indications of a real set of peaks. These parameters are the number of smoothes, the number of data points to be used in each smooth, and an estimate of the full-width-at-half-maximum for peaks in the spectrum,

The peak search subprogram has proven to be slightly conservative in that it has a tendency to locate false peaks as well as valid peaks. However, the false peaks are effectively eliminated when the fitting and evaluation routines are executed,

B. Peak Fitting Subprogram

The fitting program must provide versatility, speed, accuracy, choice of optimization, and adaptability to the photopeak spectroscopy problem,

It has been a generally accepted approach to utilize only the first derivatives of the theoretical function in the logic of fitting routines, One might expect that the second derivatives would be of little consequence, however, Gaussian functions contain significantly relevant second order derivatives which contribute to resolving complex multiplets, Test cases were run to examine and compare the qualities of first versus second order Taylors' expansions. The test case was one of high complexity which contained many hidden photopeaks in addition to possessing many spurious peaks, A comparison of the two results showed that the first order fits had a tendency to define false shapes where a large amount of scatter was present, In addition, the determination of hidden photopeaks which appeared as definite shoulders on larger peaks was generally quite poor and frequently not acceptable as shown in Figure 1. The problems with the first derivative fits were all but eliminated when second order fitting was applied and the determinations of hidden photopeaks were generally good, Thus, the criteria for selection of a fitting program was that it should employ second order derivatives in its iterative procedure,

The availability of a substantial regression analysis which may be successfully applied to the results of the fit was deemed to be very useful for evaluating the validity of each Gaussian term, Thus, evaluation of the requirements for the fitting program led to the selection of the LEARN code^(4,5) as the base from which to develop GSSLRN analysis necessary to solve some of these problems of photopeak analysis,

FIGURE 1
COMPARISON OF FIRST VERSUS SECOND ORDER FITTING

Much study^(1,2,3,6) has already been devoted to determining the best analytical function for use in fitting photopeak data. Most efforts have resulted in the selection of a Gaussian or modified Gaussian shape with some form of background continuum. Further, some accountability is generally given to the low-energy tail of each Gaussian shape such that a modified Gaussian is generally incorporated as part of the analytic function. However, GSSLRN-I has been written so as to account for this asymmetry by allowing the data to be fit with possibly more than one Gaussian contributor. This then allows the user to discriminate between true asymmetry and valid hidden photopeaks. In addition, it has allowed the application of the program to be kept general instead of being functionally tied to the photopeak problem. The result is that the analytic model for both GSSLRN-I A and GSSLRN-I B uses a sum of Gaussian terms plus a background contribution. An exponential contribution is used in GSSLRN-I A whereas a three-term polynomial is used in GSSLRN-I B.

IV. ANALYTIC MODEL

A. GSSLRN-I A

The current analytic function in program GSSLRN-I A is

$$N(\chi) = Ae^{B(\chi-\chi_o)} + \sum_{i=1}^n G_i(\chi), \quad n \leq 10 \quad (1)$$

an exponential background continuum and a symmetric Gaussian term for each of the photopeaks.

The $N(\chi)$ is the total count as a function of channel number, $Ae^{B(\chi-\chi_o)}$ is the exponential function used to describe the background continuum,

and $\sum_{i=1}^n G_i(\chi)$ is the sum of up to ten Gaussian terms.

Equation (1) is represented in GSSLRN-I A by the following:

$$N(\chi_m) = A_1 \exp \left[A_2(\chi_m - \chi_o) \right] + \sum_{i=3, JJ, 3} A_i \exp \left[-1/2 \left(A_{i+1} \chi_m - A_{i+2} \right)^2 \right] \quad (2)$$

where

A_1 is the intercept for the background continuum,

A_2 is the slope of the exponential background continuum,

A_i is the amplitude of each Gaussian function,

$A_{i+1} = 1/\sigma_i$ for each Gaussian function,

$A_{i+2} = \bar{\chi}_i/\sigma_i$ and $\bar{\chi}_i$ = mean channel; σ_i = FWHM/2.355,

JJ is the total number of parameters.

As demonstrated by Routti and Prussin⁽²⁾ and Camp⁽⁶⁾ some occasional assymetry occurs on the low-energy side of some of the photopeaks. This effect has been accounted for, as described earlier, by allowing GSSLRN-I to build in Gaussian contributors.

A test case, shown in Figure 2, did in fact reveal some of the problems associated with the low-energy assymetry. The effect, in GSSLRN-I, was that the full-widths-at-half-maximum were more nearly equal when the Gaussian contributors were allowed to be used so long as the energy interval was small.

Although the above assumption is not a particularly sound one, it nevertheless provides intensity ratios which are more reliable than those

FIGURE 2
PHOTON SPECTRUM FROM AN IRRADIATED PLUTONIUM FUEL ROD

obtained when GSSLRN-I is not allowed to assume the low-energy Gaussian contributor(s). Consequently, consistent measurement variances have been achieved for almost all intervals of fit chosen by the code. These measurement variances are normally around the expected value of one.

The code also includes tests on the measurement variance as additional criteria which must be met in order to allow searching for hidden photopeaks. Multiple fitting may be attempted on any one interval of fit in order to allow maximum resolution of multiplets in an automated manner. However, successive fitting of this type is an exception rather than a rule and normally is not done unless very complex spectra are being analyzed.

If we allow $N(\chi_o)$ to represent the count in any channel, then $\sqrt{N(\chi_o)}$ is used to represent the statistical uncertainty of that same count. While this approximation of the uncertainty may not be an accurate estimate when extremely high or low counting rates are present, it does supply statistical weights for the data which allow conservative estimates to be made of the uncertainties from the fitted parameters.

B. GSSLRN-I B

A second version of the code, GSSLRN-I B, has been written which deviates from GSSLRN-I A primarily with respect to the analytic function assumed for the background continuum. The resulting analytic function which is used to represent the data is

$$N(\chi) = A_1 + A_2(\chi_m - \chi_o) + A_3(\chi_m - \chi_o)^2 + \sum_{i=4, JJ, 3}^{JJ \leq 33} A_i \exp \left[-1/2 (A_{i+1} \chi_m - A_{i+2})^2 \right] \quad (3)$$

where A_1 , A_2 , and A_3 are standard polynomial parameters, and A_i , A_{i+1} , A_{i+2} and JJ are the same as in Equation 2.

V. CODE DESCRIPTION

GSSLRN-I has been coded to be as versatile as possible. Major segments (or links) of common interest are made available to the main program in such a manner as to minimize storage requirements and execution time. However, several subroutines that are used extensively have been allocated to the main link throughout execution. The code is made up of five major segments, excluding the main link, all of which are allocated only when needed. The segments will be described in the order in which they are called from the main program. Thus, the presentation which follows is analogous to a flow diagram of the code. Segmentation of the various links as they are allocated in GSSLRN-I is shown in Figure 3,

A. SEGMENT 1 (Input and Peak Search Routines)

This segment contains the subroutines LOAD, ANALIZ, INTEGR, OUTPUT, PKCHK, and VALLEY,

Subroutine LOAD reads input data to the program. At present, cards, magnetic tape, or data elements (DAT) on fastrand drum files may be used for inputting the data spectrum. Except for the data spectrum, a minimal amount of input cards (2 to 8) are supplied via NAMELIST⁽⁷⁾ input routines. NAMELIST is a standard input data package available on most computer systems employing FORTRAN IV, V compilers,

The subroutines ANALIZ, INTEGR, OUTPUT, and PKCHK are the peak searching and initial location routines which utilize the method described by Mariscotti,⁽¹⁾ These routines have been employed under the premise

FIGURE 3

BLOCK DIAGRAM OF PROGRAM GSSLRN-I

that the photopeaks and background continuum may be described by quantities entering into Equations (2 or 3).

If $N(\chi_m)$ is a continuous function, then the second derivative $N''(\chi_m)$ is independent of the background continuum and vanishes for any interval in which no photopeaks are present. Thus, a peak is located when $N''(\chi_m) \neq 0$.

Because of the nature of the data, one may further assume that the second derivative can be replaced by the second difference

$$S_i = N_{i+1} - 2N_i + N_{i-1} \quad (4)$$

which will also be different from zero in the vicinity of a peak as is $N''(\chi_m)$. The standard deviation of S_i is given by

$$F_i = (N_{i+1} + 4N_i + N_{i-1})^{1/2} \quad (5)$$

Mariscotti has shown that the optimum choice of input parameters for peak locations are

INTEG = 5; number of smoothes to be used and

LENT = $0.6 \cdot \text{FWHM}$; the number of channels to be used in each smooth,

As explained earlier, this approach⁽¹⁾ tends to be somewhat conservative. Therefore, an effort was made to increase the sensitivity of the second difference. An empirical approach was found which suggested that only the second difference needed to be modified. The result was that Equation (4) was modified to be

$$S_i = -0.1(-N_{i-3} - N_{i-2} + N_{i-1} + 2N_i + N_{i+1} - N_{i+2} - N_{i+3}) \quad (6)$$

where S_i is expressed now as a weighted second difference. Except for the sign and magnitude change, Equation (6) is the weighted second

difference described by Routti and Prussin,⁽²⁾ This method has resulted in increased sensitivity in addition to better identification of real peaks, It should be noted, however, that the weighted second difference has only been applied to data spectra whose full-widths-at-half-maximum range from two to twenty channels,

The peak search routines also provide the initial interval of fit for each peak, The range of the interval is selected by the user. However, it is inspected and possibly modified by other routines so as to select those peaks which are sufficiently close and group them as "sets" before any attempts are made to fit the data,

Subroutine VALLEY's only function is to compute check points on or between peaks for purposes of interval selection,

B. SEGMENT 2 (Input Parameters and Peak Grouping Routines)

This segment of the code contains the subroutines PUTIN, LIMITS, SPLIT, SPLICE, and LIST, It provides the means for computing initial estimates of the fitting parameters, minimizing input requirements, optimizing the interval of fit, and supplying some input values⁽⁵⁾ which would normally have been required by the user,

Subroutine PUTIN is written to supply initial estimates for the fitting parameters and other parameters specifically related to the iterative properties of program LEARN,^(4,5) One of these parameters is the variable known as RATE, This parameter controls the magnitude of the incremental change of direction for each of the quantities in the iterative steps leading to convergence. RATE appears to be functionally tied and sensitive to FWHM (full-widths-at-half-maximum) and the displacement

between the means of each peak when fitting sums of Gaussians to multiple peaks. The amount of coupling (or overlapping) between Gaussians in a multiplet is what determines the optimum value for RATE. In tightly coupled problems, this quantity can reduce the number of Iterations required to obtain convergence by a significant factor. Convergence is frequently sporadic when RATE is not properly chosen.

Subroutines LIMITS, SPLIT, and SPLICE are called from PUTIN and are designed to choose a more precise interval of fit and to group the photopeaks in sets for fitting. Initially only a spatial grouping of peaks was attempted. However, experience proved that some valid photopeaks were discarded because of their relative intensities and/or criteria on the allowable displacement from other photopeaks. In these routines, tests are made to determine if estimates of relative intensities could suggest further splitting of the set. This test was deemed necessary because the fitting routines have a tendency to smear small peaks into the background continuum. If such peaks are present, then they are separated into different intervals of fit. In addition, if a split is made, it is done in such a way as to preserve data within the modified interval which might contain a hidden photopeak. As a result, it is possible to re-apply data, which exists in the valleys, to more than one set for fitting purposes.

The method of group and interval selection used above has proven to be substantially stable, and more importantly, it provides a degree of consistency for the total spectrum with respect to the degree of freedom used in each fitting attempt. It also results in the measurement variances for the entire spectrum being relatively consistent. Finally, the measurement variance may be used in testing to decide if any particular set of Gaussian peaks has been totally resolved.

With subroutine LIST the initial input estimates that are supplied primarily by PUTIN are printed out,

C. SEGMENT 3 (Fitting and Recycling Routines)

This segment contains the subroutines MINMAX, DOUBT, SADDLE, PUTOUT, MISFIT, WORTH, WIT, WITTY, ADJ1, and ADJUST. It is the heart of GSSLRN-I. It contains the fitting logic, saddle point logic, theory-measurement correlation, regression analysis, variance-covariance matrices, evaluation of fitted Gaussian shapes, and recycling procedures,

Subroutine MINMAX contains the iterative procedures which are based on second order Taylors' expansions in the Newton-Raphson iteration scheme, ⁽⁴⁾

The principal function of DOUBT is to provide the variance-covariance subset matrix which contains the measurement uncertainties of the fitted parameters and a measure of the measurement variance. Subroutine DOUBT also calls SADDLE to provide an analysis relevant to saddle conditions which could result from the iterative procedure. Information regarding possible saddle conditions, a listing of the best set of fitted parameters, and the measurement variance is supplied,

Subroutine PUTOUT converts the fitted function parameters to values which can be recognized by the user.

Subroutine MISFIT is available upon option to provide a theory-measurement correlation printout. When MISFIT is called, no on-line plotting options (NPAP = -1) are available as they would represent redundant information,

The primary function of subroutine WORTH is to allow the user to initiate an evaluation (regression analysis) of the fitted parameters. This evaluation is an automatic feature in GSSLRN-I and is applied to

each Gaussian term. The worth, or contribution to the total fit of each Gaussian term is used as one of a series of tests to decide acceptability of each Gaussian term. The function of this regression analysis has effectively proven itself as a necessary aid when coupled Gaussian multiplets are to be resolved.

Subroutines WIT and WITY are used to make the final decisions on the fitted Gaussians and possible recycling with more or less Gaussian terms.

Basically, the function of subroutine WIT is that of screening the Gaussian terms to determine if they meet acceptable criteria. If not, then they are flagged as false peaks and discarded from the total sum of Gaussian terms in order that a refit can be made. Once all peaks are flagged GOOD, then the code will proceed to subroutine WITY.

In subroutine WITY at least one search is attempted for hidden peaks. The search is performed on the basis of the quality of the fit (i.e., the measurement variance). Two quantities, at the user's discretion, are used to validate the search. The first, AMIN(98), is used to eliminate statistical fluctuations which might be recognized as peaks. The AMIN(98) value is the minimum number of sequential data points whose deviations from the fit have the same algebraic sign, and whose deviations are greater than the quantity AMIN(99) times the square root of the measurement variance (i.e., the root-mean-square-misfit). This is shown as the following:

$$\text{If } \left[\left(\frac{Y-YM}{\sqrt{YM}} \right)_i \leq - \text{AMIN}(99) * \sqrt{Q(8)} \right]$$

where $\left(\frac{Y-YM}{\sqrt{YM}} \right)_i$ represents the deviation at each data point, and Q(8) is

the measurement variance; and if the test is true for at least AMIN(98) sequential data points, then estimates are made to attempt to build in a hidden peak in addition to those already fitted.

Because of the logical procedure in the program and the characteristics of least-squares fitting when not all of the peaks have been fitted, the above test on the deviations must demand that they be only negatively valued rather than choosing all of those whose absolute values were greater than the multiple of the measurement variance. Otherwise, false peaks would be identified. The peak(s) already fitted are not required to maintain their fitted parameters. These parameters are varied along with those parameter estimates for the hidden peaks when the code recycles for another fit.

Provided the code (GSSLRN-I) successfully builds-in and fits a hidden peak(s), then a second check is made on the measurement variance to determine if all the peaks in the interval of fit have been located and fitted. This second attempt at locating hidden peaks will be initiated under the following criteria:

For GSSLRN-I A; if $[(Q(8) - (MSETS + 2) - .67) \geq 0]$, where MSETS is the number of Gaussian terms- then another search for hidden photopeaks is attempted.

For GSSLRN-I B; if $\left[\frac{Q(8) - MSETS}{MSETS} > 10 \right]$, then another search is allowed.

Under any prior circumstances, if an attempted fit fails. then GSSLRN-I will recover the last set of acceptable fitted parameters. This process of locating and fitting hidden photopeaks is obviously dependent upon how well Gaussian shapes approximate the photopeaks.

In addition, the quantity RATE, referred to earlier, plays an important role when recycling with estimates for hidden peaks. It has been found, empirically, that a good rule-of-thumb for the choice of RATE under recycle conditions is the following:

$RATE \triangleq FWHM/|DIFF|$ if $0.5 \leq RATE \leq 1.0$. where DIFF is the displacement of the hidden peak from the fitted mean of the closest neighboring Gaussian.

Following completion of a successfully fitted Gaussian "set", the intensity of each peak is analytically computed from $I_k = A_i/A_{i+1} * \sqrt{2\pi}$, where A_i and A_{i+1} are the Gaussian amplitude and $1/\sigma_k$, respectively, for the k^{th} peak. The uncertainty of each intensity value is defined as

$$\delta I_k = \left\{ \frac{2\pi}{A_{i+1}^2} \left[\overline{(\delta A_i)^2} \frac{2A_i}{A_{i+1}} \overline{(\delta A_i \delta A_{i+1})} + \left(\frac{A_i}{A_{i+1}} \right)^2 \overline{(\delta A_{i+1})^2} \right] \right\}^{1/2} \quad (7)$$

where $\overline{(\delta A_i)^2}$ and $\overline{(\delta A_{i+1})^2}$ are the measurement variance uncertainties and $\overline{(\delta A_i \delta A_{i+1})}$ represents the cross-correlation term, all of which are obtained from the variance-covariance matrix mentioned earlier.

Subroutines ADJ1 and ADJUST are used as supplements to WIT and WITTY, respectively, for purposes of readjusting the interval of fit when peaks are discarded or built-in.

D. SEGMENT 4 (CALCOMP Plotting Routines)

This segment contains the subroutines CONTRL, MAPS, PLOT, ARTIST, LOGAXS, PLTTER, SCLE, and SHUTLE. This segment of GSSLRN-I provides two basic options for creating plots on a Calcomp plotter.

The first option, NPAP = 1, allows the user to obtain plots which are generated from each successful fit. Each of these plots contains the count per channel, its assumed error bar, the fitted curve, the root-mean-square deviation envelope, a plot of each resolved Gaussian term, and finally the fitted numerical values for the area, full-width-at-half-maximum, mean channel, and energy of each peak.

The second option, NPAP = -2, allows the user to obtain a plot of the measured spectrum (up to 4096 channels).

Subroutine `CONTROL` is used with the first option only and provides automatic scaling for linear or semi-logrithmic graphs.

Subroutine `MAPS` is used by both options and contains the basic plotting logic for `GSSLRN-I`,

Subroutine `PLOT` is used to provide scale factor changes such as linear or semi-logrithmic conversion.

Subroutine `ARTIST` provides the appropriate labeling of scales for both options,

Subroutine `LOGAXS` is used to generate logrithmic scales of any size,

Subroutine `PLTTER` is the controlling routine when the spectrum plots are generated (i.e., `NPAP = -2`).

Subroutine `SCLE` computes the plotting ranges for `PLTTER`.

Subroutine `SHUTLE` provides automatic linear scaling for both options,
E. SEGMENT 5 (On-line Plotting Routines)

This segment contains the subroutines `SETUP`, `IMAGE`, `SORAS`, `CHAR`, and `SORT`. This segment of `GSSLRN-I` is used to supply the plots which may be obtained on-line with the printout of each successful fit. Each plot will contain the count(*), and the fit(-) on a plot of count rate versus channel number. If the count and the fit at the same channel fall on the same coarse grid location, then the point will be plotted as a (\$).

The use of these routines is somewhat limited in that some are written in machine language and are not always adaptable to computer systems other than the UNIVAC-1108. Therefore, no detailed explanation will be given,

F. Output Quantities

Finally, a summary is printed which contains the following information for each successfully fitted peak:

- Mean channel
- Mean channel uncertainty
- Energy
- Energy uncertainty } optional
- Full-width-at-half-maximum
- FWHM uncertainty
- Net area (analytically computed)
- Net area uncertainty
- Relative area (normalized to any number)
- Measurement variance for each Gaussian set.

G. Relative Differences Between GSSLRN-I A and GSSLRN-I B

Further improvements or modifications are listed below;

- Contrary to GSSLRN-I A, the interval of fit selected by the user may be much larger when executing GSSLRN-I B so as to define (or fit) the background continuum better. Experience thus far has suggested that $\bar{\chi}_1$ (mean channel) $\pm 3 \cdot \text{FWHM}$ is an optimum choice for fitting when using GSSLRN-I B, whereas $\bar{\chi}_1 \pm 2 \cdot \text{FWHM}$ is optimum for GSSLRN-I A.
- The somewhat random addition of Gaussian contributors which are present with GSSLRN-I A have been essentially eliminated when using the polynomial for fitting the background. This condition has resulted in better definition of intensities when multiplets are fitted. In addition, the full-widths-at-half-maximum appear to be even more consistent within any energy interval,

- Measurement variance quantities tend to be smaller in addition to suggesting the presence of hidden photopeaks on a more affirmative basis when using GSSLRN-I B.
- The input quantities AMIN(98) and (99), described in the input requirements, need not be defined with the precision demanded by GSSLRN-I A in order to locate hidden photopeaks with GSSLRN-I B.
- The polynomial continuum allows the code to fit Gaussian shapes in the neighborhood of Compton edges,

Table 1 lists a set of fitted quantities taken from data in Figure 2 which shows a comparison of fits made with both codes,

In conclusion, the properties, both input and output, of GSSLRN-I B seem to suggest that this version of the code is probably more reliable and definitely more consistent in the way it fits Gaussian functions to data from a photopeak spectrum. However, it should be noted that both versions of GSSLRN-I are written such that the code need not be modified when more precise equipment becomes available,

VI. CONCLUSIONS

Program GSSLRN has been used to analyze photopeak spectra of high complexity which contained many unknown components. One such spectrum, shown in Figure 2, illustrates the complexity of data measured and analyzed. The spectrum in Figure 2 was used routinely as a test case for GSSLRN-I because of the high rate of coupled multiplets and hidden photopeaks. Illustrations representing some of these resolved multiplets are shown in Figures 4 and 5,

TABLE I
COMPARISON OF THE RESULTS OF GSSLRN-I A AND GSSLRN-I B
 Fitted data are from the test spectrum shown in Figure 2.

<u>Mean Channel (1A)</u>	<u>Mean Channel (1B)</u>	<u>FWHM (1A)</u>	<u>FWHM (1B)</u>	<u>Area (1A)</u>	<u>Area (1B)</u>	<u>Area (1B) Area (1A)</u>	<u>Total Area (by hand)</u>
454.62	454.59	3.562	3.395	96 499	90 033	0.933	
467.86	467.86	3.609	3.582	898 746	890 414	0.991	1 037 808
551.66	551.48	3.469	3.787	115 527	103 819	0.899	
556.13	-	4.350	-	7 383	-	-	
562.07	562.12	3.608	3.228	29 982	23 541	0.785	
567.16	567.16	3.644	3.639	349 360	346 586	0.992	503 587
579.76	579.76	2.950	3.071	4 115	4 334	1.053	**
-	599.10	-	4.218	-	10 688	-	
602.86	602.90	3.776	3.692	304 665	300 769	0.987	310 501
634.33	634.33	3.700	3.695	34 001	34 011	1.0003	34 799
659.27	659.32	3.798	3.679	184 792	176 015	0.953	190 175
688.63	688.68	3.595	4.108	294 081	234 469	0.797	
696.81	696.78	3.772	3.850	816 930	840 394	1.029	1 101 893
723.88	723.88	3.819	3.793	69 907	69 157	0.989	
729.24	729.20	3.449	3.215	6 466	5 729	0.886	
737.32	737.36	3.602	3.310	5 833	5 118	0.877	84 232
793.97	793.96	3.860	3.794	11 484	11 212	0.976	
804.05	804.10	3.891	3.657	2 046	1 841	0.900	11 029
851.62	851.69	4.209	4.206	1 094	1 101	1.006	1 150
-	912.47	-	3.058	-	609	-	**
953.46	953.46	4.108	4.085	31 316	31 075	0.992	34 665
1023.55	1023.54	4.044	4.147	7 580	7 899	1.042	7 820
1056.11	1056.09	4.380	4.252	4 933	4 731	0.959	
1060.30	1060.29	2.603	2.688	1 206	1 258	1.043	
1064.14	1064.15	4.026	3.975	7 038	6 890	0.979	13 672
1083.45	1083.41	3.907	4.050	1 068	1 152	1.079	**
1093.08	-	3.585	-	244	-	-	**

*The resolved areas of the peak in the set are not necessarily correct because of Gaussian contributors.

**Hand calculations not available.

EXAMPLES OF RESOLVED MULTIPLETS

FIGURE

FIGURE

Although the code has been used only on a limited number of spectra, (v200) the indications (i.e., measurement variance, determinations of means and areas, etc.) are that the second derivatives play an important role in the analysis of photopeak spectra. This does not imply that the second derivatives are always essential in fitting codes, but does indicate that the characteristics of resolved Gaussian shapes can be improved when applying this technique,

Except for efficiency calibrations, the code can be used routinely to analyze spectra of varied complexity. In addition, input requirements are at a minimum and define the major options to be executed. These input quantities are also used to define the statistical criteria necessary for locating hidden photopeaks.

Experience with program GSSLRN-I has demonstrated that the measurement variance can be utilized to provide a meaningful statistical criteria for the resolution of multiplets. Thus far, the consistency of the measurement variance and the degrees-of-freedom have indicated with good reliability the existence of well hidden photopeaks.

VII, INPUT REQUIREMENTS

The input requirements for the codes GSSLRN-I A and GSSLRN-IB are identical and they utilize the NAMELIST⁽⁷⁾ utility package which is available with most FORTRAN IV or V compilers. Knowledge of NAMELIST and its use is assumed,

o Required Input

<u>Name</u>	<u>Description</u>
IMIN	<p>This number defines the beginning channel of either the peak search and/or the fitting analyses. Because of the method of initial peak location, this value should be approximately $IMIN \hat{=} \bar{X}_1 - (3*FWHM)$, where $\bar{X}_1$ is the center of the first peak,</p> $1 \leq IMIN \leq (2048 - 3*FWHM)$
MAX	<p>This number defines the last channel to be used for either the peak search and/or the fitting analyses,</p> $IMIN < MAX \leq 2048 \text{ when } NPAP \neq -2;$ $IMIN < MAX \leq 4096 \text{ when } NPAP = -2,$
INTEG	<p>This value is $\pm N$, where N represents the number of times that the measured data will be smoothed (or averaged) in the peak search,</p> <p>If $INTEG = -N$, the user may execute successive cases for the same spectrum in order to optimize this value without supplying the spectrum counts more than once,</p> <p>If $INTEG = 0$, no smoothing is applied,</p> <p>If $INTEG = N$, then N number of smoothes will be applied and the code will then proceed to the fitting analyses,</p> <p>Optimum value for INTEG is usually 5,</p>

● Required Input

<u>Name</u>	<u>Description</u>
LENT	<p>This value defines the number of channels to be used in each smooth, LENT may be optimized by allowing INTEG to be a negative value,</p> <p>Optimum value is usually $LENT \doteq 0.6 * FWHM$.</p>
FWHM	<p>This number approximates the value of the full-width-at-half-maximum of the peak(s) located between IMIN and IMAX,</p>
NPAP	<p>NPAP is a control integer which dictates major options of execution-</p> <p>= -2; Spectrum plots are generated, (IMAX $\leq$ 4096 channels,)</p> <p style="padding-left: 40px;">No other NPAP options should be executed when this option is applied.</p> <p>= -1; On-line computer plots are generated showing the measured data (* symbol) and the fitted results (- symbol) for each channel in the interval of fit,</p> <p>= 0; A printout of the theory-measurement correlations for each channel, as they are computed in sub-routine MISFIT, is obtained</p> <p>= 1; Automatically scaled Calcomp plots of each successfully fitted group of Gaussian shapes are obtained showing the measurement, measurement uncertainty, the best fit and its root-mean-square deviation envelope, each resolved Gaussian shape</p>

<u>Name</u>	<u>Description</u>
	<p>excluding the background continuum, and fitted numerical quantities such as the mean, full-width-at-half-maximum, area, and energy,</p> <p>= 2; Only input and fitted information are obtained, Except when NPAP = -2, a summary table of fitted quantities is included with all NPAP options,</p>
LIP	<p>This quantity is supplied as a control feature for users wanting only the summary of fitted information.</p> <p>= 0; All of the above NPAP options are available as described,</p> <p>= 1, and NPAP # -2; the printout will consist of the peak search and the summary of fitted information.</p>
AMIN(9 7)	<p>AMIN(97) partially defines the initial interval of fit. (ie $\bar{x}_1 \pm \text{AMIN}(97) * \text{FWHM}$ in channels),</p>
AMIN(9 8)	<p>This quantity, combined with the test on AMIN(99), defines the minimum number of required differences ($Y_{\text{calc.}} - Y_{\text{meas.}}$) which must occur sequentially, with the same algebraic sign in order to validate location of hidden photopeaks,</p> <p>$100 \geq \text{AMIN}(98) \geq 2$,</p>
AMIN(99)	<p>This quantity is the factor which is multiplied by the square root of the measurement variance in order to establish a limiting criteria for recognizing hidden photopeaks*</p>

Tests on both AMIN(98) and AMIN(99) must be satisfied in order to validate the location of hidden photopeaks,

<u>Name</u>	<u>Description</u>
AMIN(100)	This quantity can be used as the value desired for relative intensity normalization, IF AMIN(100) is not supplied, then the program will normalize all intensities to the largest intensity calculation of the entire spectrum.

The data input subroutine **LOAD** will accept data for up to twelve channels per card or tape record,, This allows the user the freedom of choice to read data by blocks if necessary, Therefore, the input variable **LOT** has been used to define the necessary input characteristics of his spectrum.

LOT(1,9)	This is the first channel to be read,
LOT(2,9)	This is the last channel of each block, card, or record,
LOT(3,9)	This defines the total number of blocks, cards, or records which are to be read,
LOT(4,9)	Defines a constant channel number which can be used to shift the data. This is done only when the summary is printed, Preset to zero, not required as input,
LOT(5,9)	A control integer used to designate one of two types of printout on the summary page, = 0; no energies are computed, = 1; energies and their uncertainties are included in the summary.

Preset to zero, not required as input,
 If LOT(5,9) = 1 then UGEN and UEXP can be used as additional input values for converting the fitted means (channels) to energies, Normally, these are values obtained from a calibration fit to a straight line which passes through known energy levels,

<u>Name</u>	<u>Description</u>
UGEN	This is the slope of the straight line approximation, Preset to 1.0, optional input,
UEXP	This is the intercept of the straight line approximation, Preset to 0., optional input,
LOT(6,9)	Logical unit specification for reading the spectrum counts, = 2 or 5; cards are used as the input media, = 1,4,7,9,10,11,12,13, or 15; magnetic tape is the input media, = 25,26,27,28, or 29; DAT elements on cards or magnetic tape are inputed and stored as data elements on the computer drum,

DAT elements may be inputed via cards or magnetic tape. If magnetic tape is used, then they must be introduced via the "complex utility routines", CUR, directives. In addition, if DAT elements are used then there may be a maximum of "ten" successive cases (separate spectrums) in any one computer execution. Further, they must be identified in the following manner and be in the same order as the successive cases;

V DAT NAME/VER, 0

V DAT NAME/VER, 1

etc

V DAT NAME/VER, 9

LOT(6,9) is preset to 2 for card input media,

Optional input, not required,

- Optional Input

The following input variables are required when using any Calcomp plotter options.

<u>Name</u>	<u>Description</u>
MAP	<p>Due to the automated plotting specialties written for GSSLRN-I. the function of MAP has been limited from that which it was normally used in program LEARN^(4,5) to the following choices:</p> <p>= 0; No plotting will be attempted.</p> <p>=-1, and NPAP $\neq$ -2, plots for each successfully fitted peak will be generated.</p> <p>=-1. and NPAP = -2; plots of measured spectrums may be generated,</p>
FCIR	<p>This is a special scaling feature which allows the user to magnify or reduce the total size of any desired graph, Normally FCIR = 1.0.</p>
NPLOT	<p>NPLOT specifies one of two scaling features,</p> <p>=1; Semi-logarithmic scales are generated,</p> <p>=2; Linear scales are generated,</p>
MARK	<p>This quantity specifies which Calcomp symbol is to be used to designate the measured data.</p> <p>When NPAP $\neq$ -2, MARK must be positive in value,</p> <p>When NPAP = -2, refer to "Special Features"</p>
CYCLE	<p>This quantity specifies the maximum height, in inches, of each plot,</p> <p>When NPAP $\neq$ 2; $2 \leq \text{CYCLE} \leq 10$</p> <p>When NPAP = -2. refer to "Special Features."</p>
KK	<p>RK is a control integer used to specify automatic scaling features.</p> <p>When NPAP $\neq$ -2, KK = 1. Not required input,</p> <p>When NPAP = -2, refer to "Special Features,"</p>

<u>Name</u>	<u>Description</u>
LINE	Control integer for NPAP = -2 option; refer to "Special Features," When NPAP # -2, LINE = 2. Not required input,

- Special Features

The following list of input variables have special functions which are available when NPAP = -2,

<u>Name</u>	<u>Description</u>
MAP	MAP = -1 is mandatory for each case,
MARK	This quantity specifies which Calcomp symbol is to be used to represent the measured data, MARK may be positive or negatively valued, If MARK = + in a successive case execution, each case (or spectrum) will be plotted individually. If MARK = -, then each successive plot of a spectrum will be superimposed on the same graph up to and including the case where MARK = +.
KK	This is a control integer used to specify automatic scaling, = 1, then no automatic scaling is attempted, and the variable ZDZSDS is required input data, =-1, then the program will automatically scale each plot and the variable ZDZSDS is not required,
LINE	This is a control integer used to specify line or symbol plots. = 2, yields a plot with lines drawn between each data point, = -2, yields a plot with only data symbols,

<u>Name</u>	<u>Description</u>
CYCLE	<p>Maximum height of plot allowed in inches,</p> <p>If $KK = 1$ and $NPLOT = 1$, then CYCLE defines the height in inches of each logarithmic cycle.</p> <p>If $KK = 1$ and $NPLOT = 2$, then CYCLE has no function.</p> <p>If $KK = -1$ and $NPLOT = 1$ or $NPLOT = 2$, then CYCLE defines the maximum height in inches of the total graph,</p>
TITL1(1) = 54H	These four input quantities are available so as to
TITL2(1) = 54H	specify four lines of alpha-numeric information
TITL3(1) = 54H	which identifies each spectrum plot- They are plotted
TITL4(1) = 54H	in the lower left corner of each graph.
ZDZSDS	<p>These quantities are used to specify plotting ranges,</p> <p>$= ZDZSDS (L,K,M)$; $L = 1, 6$, $K = 1, 2$; $M = 1$.</p> <p>If $KK = -1$, these quantities are not required input,</p> <p>Otherwise, they are used in the following manner:</p> <p>Example for a plot ranging from 1 to 1×10^6 on the Y-axis over a span of 24 inches and the X-axis ranging from 0 to 4096 channels over a span of 40.96 inches.</p> <p>Y-axis definition when $NPLOT = 1$:</p> <p>$ZDZSDS(1,1,1) = 1., 0., 1. + 6, 0., 0., 24000.,$</p> <p>Y-axis definition when $NPLOT = 2$.</p> <p>$ZDZSDS (1,1,1) = 0., 0., 1. + 6, 0., 0., 24000.,$</p> <p>X-axis definition:</p> <p>$ZDZSDS(1,2,1) = 0., 0., 4096., 0., 0., 40960.,$</p> <p>The second and fifth values for each axis card are always zero,</p> <p>Further explanation of the variable ZDZSDS may be obtained from Reference 5,</p>

VIII. ACKNOWLEDGMENTS

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APPENDIX A
PROGRAM EXECUTION

APPENDIX A

Program Execution

As was mentioned earlier, there are optional input requirements available; however, sample execution of only one type will be presented,

Example for executing GSSLRN-1 B on the UNIVAC-1108 system and generating the output shown in Appendix B is as follows:

```
V  RUN      5,CUS      ,5,125      GD SEYBOLD      GSSLRN-1B
VR  ASG H=(,NH,AT)-----NECESSARY WHEN CALCOMP PLOTS ARE USED.
V  XQT CUR
    IN FT0100
V  MSG  **CALCOMP PLOTTER INSTRUCTIONS, IF USED**
V  XQT GSSLRN
    $LEARN IMIN=424, IMAX=1130, INTEG=5, LENT=3, FWHM=5., NPAP=-1, LIP=1,
    AMIN(97)=3., 2., 1., 1.+6, LOT(1,9)=1, 256, 8, 0, 1, 2,
    UGEN=1.1097, UEXP=-7.535, $
SPECTRUM DATA GOES HERE (USING A 12I6 FORMAT, OR LESS)
V  FIN
```

Expected execution time will range from two to seven seconds per peak depending on the frequency of hidden peaks.

APPENDIX B

SAMPLE PROBLEM

START ARRAY	END ARRAY	NUMBER SMOOTHES	POINTS IN SMOOTH	FULL WIDTH HALF MAX	INTERVAL OF FIT
424	1130	5	3	5.00	3.000

ESTIMATE OF LOCATED PEAKS AND RELATIVE INTENSITIES

PEAK NUMBER	POSITION	RELATIVE AREA	PEAK FLAG	STARTING CHANNEL	ENDING CHANNEL	KA
1	454 _a 57	_a 10423	1	440	470	452
2	467 _a 89	1.00000	1	453	483	466
3	551.47	_a 11144	1	536	566	549
4	567.13	_a 37282	1	552	582	565
5	579 _a 99	_a 00440	1	565	595	578
6	602.90	_a 32879	1	588	618	601
7	634 _a 30	_a 03708	1	619	649	632
8	659.26	_a 19817	1	644	674	657
9	687 _a 96	_a 11907	1	673	703	686
10	696 _a 89	_a .84815	1	682	712	695
11	723.90	_a .07114	1	709	739	722
12	737 _a 56	_a .00520	1	723	753	736
13	793 _a 96	_a 01201	1	779	809	792
14	804.41	_a .00171	1	789	819	803
15	821.60	_a 00039	1	807	837	817
16	851 _a 73	_a .00112	1	837	867	849
17	912.76	_a 00078	1	898	928	911
18	953 _a 50	_a 03212	1	938	968	951
19	1008.63	_a 00047	1	994	1024	1003
20	1023.57	_a 00787	1	1009	1039	1021
21	1055.64	_a 00254	1	1041	1071	1054
22	1064.20	_a 00553	1	1049	1079	1062
23	1083.44	_a .00111	1	1068	1098	1081
24	1093.37	_a 00024	1	1078	1108	1092

PLUS OR MINUS 3.000+00 *FWHM IS THE INITIAL INTERVAL OF FIT
 2.000+00 POINTS IN SEQUENCE ARE REQUIRED TO LOCATE SHOULDERS
 1.000+00 IS THE MULTIPLE RMS REQUIRED TO LOCATE SHOULDERS

TIME 1.4201009+00M

S U B R O U T I N E T A L L Y

SUMMARY OF GAMMA PEAK INFORMATION (FITTED PEAKS ONLY)

PEAK	MEAN CHANNEL	MEAN CHANNEL ERROR	ENERGY	ENERGY ERROR	FWHM (WIDTH)	FWHM (ERROR)	AREA (NET)	AREA (ERROR)	RELATIVE AREA	MEASUREMFNT VARIANCE
1	454.5937	3.1483278-03	496.9276	3.4936994-03	3.395360	1.2024429-01	90033.21	3227.1	9.00332-02	
2	467.8618	3.7133925-04	511.6512	4.1207516-04	3.581968	1.8921001-02	890414.3	4839.9	8.90414-01	14.378
3	551.4852	4.1552280-03	604.4482	4.6110564-03	3.787361	8.9285295-02	103818.6	2543.9	1.03819-01	
4	562.1210	5.1362628-02	616.2507	5.6997108-02	3.228377	2.9128061-01	23540.60	2240.6	2.35406-02	
5	567.1598	3.0179866-03	621.8422	3.3490597-03	3.638967	3.7288775-02	346586.4	3469.1	3.46586-01	11.827
6	579.7628	1.6108457-02	635.8278	1.7875554-02	3.071035	3.8205709-01	4334.249	528.58	4.33425-03	1.3433
7	599.1002	6.8227673-01	657.2865	7.5712247-01	4.217504	1.2447852+00	10688.14	4665.8	1.06881-02	
8	602.9030	1.7831788-02	661.5064	1.9787935-02	3.692461	3.1316389-02	300768.9	4422.6	3.00769-01	4.4194
9	634.3276	1.0835163-03	696.3783	1.2023780-03	3.695229	5.8799575-02	34011.49	568.19	3.40115-02	2.3164
10	657.4395	9.4781303-02	722.0256	1.0517881-01	8.518189	9.0274478-01	16691.98	2706.7	1.66920-02	
11	659.3151	2.8028240-03	724.1069	3.1102938-03	3.679170	2.6816654-02	176015.2	2182.5	1.76015-01	2.2296
12	688.6835	5.1106551-03	756.6971	5.6712938-03	4.108149	9.5360141-02	234468.8	5334.0	2.34469-01	
13	696.7813	1.6931742-03	765.6832	1.8789154-03	3.849606	3.4535297-02	840393.5	8485.9	8.40393-01	74.240
14	723.8858	4.1618524-03	795.7610	4.6184076-03	3.793399	3.7882926-02	69157.21	648.14	6.91572-02	
15	729.1954	3.2440887-02	801.6532	3.5999651-02	3.215309	2.4640517-01	5728.755	453.94	5.72876-03	
16	737.3580	1.6469487-02	810.7112	1.8276189-02	3.309708	2.2196886-01	5118.151	388.04	5.11815-03	2.9949
17	793.9639	4.1621486-03	873.5268	4.6187362-03	3.793669	8.1693814-02	11212.32	261.07	1.12123-02	
18	804.1023	2.8450771-02	884.7773	3.1571820-02	3.656904	3.2977737-01	1840.951	200.18	1.84095-03	1.1796
19	851.6924	3.4181605-02	937.5880	3.7931326-02	4.206469	6.2892381-01	1100.731	198.93	1.10073-03	1.2426
20	912.4710	3.5145240-02	1005.034	3.9000672-02	3.058277	7.1339728-01	609.3678	152.34	6.09368-04	1.6994
21	953.4611	4.4816904-03	1050.521	4.9733318-03	4.084921	6.1705598-02	31075.01	505.95	3.10750-02	4.3491
22	1009.616	5.9239075-02	1112.836	6.5737600-02	14.58020	2.4570504+00	2708.305	815.50	2.70830-03	
23	1023.543	4.8637757-03	1128.291	5.3973318-03	4.146860	9.0382849-02	7898.738	193.51	7.89874-03	1.2535
24	1056.094	6.4257915-02	1164.413	7.1307007-02	4.252247	2.4674259-01	4730.561	285.07	4.73056-03	
25	1060.291	3.9883810-02	1169.070	4.4259064-02	2.688330	4.5613387-01	1258.467	302.43	1.25847-03	
26	1064.154	5.2746862-02	1173.356	5.8533192-02	3.975004	1.5901948-01	6889.615	291.71	6.88961-03	1.3107
27	1083.407	2.5137863-02	1194.722	2.7895486-02	4.050375	3.9896264-01	1152.155	145.54	1.15215-03	.75325

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