CALCULATIONS OF THE FULL WIDTH AT HALF MAXIMUM IN ENERGY SPECTRA

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ABSTRACT

Four different methods for calculating full width at half maximum (FWHM) are presented and solved by computer generated pseudorandom normal distributions of known parameters. The four applied methods employ : the definition of FWHM, the relation between FWHM and the area under a Gaussian, the second moment of the peak, and the least squares fit of the logarithm of the distribution to a parabola. The dependence of the error in the calculated FWHM on the Gaussian parameters, amplitude, mean and variance is presented and discussed for each method. A comparison among the methods shows the superiority in accuracy of the second moment method.

Keywords: Energy spectrum, Resolution, Peak width.

1. INTRODUCTION

The full width at half maximum (FWHM) of the peak in an energy spectrum is a conventional measure to the detector energy resolution or, generally speaking, the spectrometry system energy resolution. There are a number of potential sources of fluctuation in the response of a given detector which result in broadning of the energy pulses and consecuently imperfect energy resolution.

These include source of random noise within the detector and instrumentation system, discrete channels of the multichannel analyser (MCA) which is the common instrument employed for energy distribution measurements and statistical noise arising from the nature of the measured signal itself.

Under these conditions, the determination of FWHM of the peaks in the spectrum as well other spectrum parameters is not accurate and the result may depend on the method used for calculating these parameters.

Experimentally FWHM is measured at two levels : with MCA during or after data accumulation, and with spectrum analysis programs, usually running on a computer to which the data have been transferred from MCA. The MCA usually employs simple algorithms for calculating spectrum parameters, / 1 /.

More sophisticated algorithms can be used by programs runing off-line, and which are more time consuming.

The evaluation of the accuracies of some of these methods is the object of this paper. Four of these methods are presented, two of which belong to the simple and fast class, and the two to the other class.

The methods are applied to computer generated pseudorandom normal distributions of known parameters,/ 2 /, and the error in the calculated value of FWHM using each of the four methods is presented. Since the treatment is carried out with random distributions, multiple Gaussians are processed for every set of parameters and the results are presented in terms of averages and standard deviations.

It is also interesting to study the sensitivity of the FWHM value to the distribution parameters when the distribution is smooth, i.e., replacing the randomly generated normal distribution with smooth Gaussian of the same parameters and applying the same methods to calculate FWHM.

2. PARAMETERS OF CALCULATIONS

A computer program has been written to enable the generation of the Gaussians and the calculation of the FWHM for each. The parameters the program uses for generating a Gaussian are : The type of

Gaussian [either random (G_1) or smooth (G_2)], the mean m, the variance s^2, and the number of counts N in the most probable channel (MPC),/3/.

G_1 Gaussians represent energy distributions encountered in common radiation measurements. They are generated by a subroutine which returns a set of pseudorandom numbers normally distributed. For a Gaussian with desired m, s^2 and N, the subroutine is called to return a total of $Ns(2\ p)^{1/2}$ numbers. To achieve desired distribution these numbers are then scaled by s and shifted by m, / 2 /.

This distribution differes from some realistic distributions in the lack of any background counts in it. The reason for not adding background counts is the wish to isolate the influence of the FWHM calculation methods on FWHM accuracy from the influence of the error introduced by some background subtraction method.

G_2 Gaussians are generated by substracting scaled values of erf(x), (error function), for values of x which represent, after proper scaling and shifting, consecutive channels.

The following set of parameters was used :

N : 100, 300, 1000, 3000, 10 000 counts,

s : 2, 3, 4, 5, 6, 8, 10 channels,

m : Channel 100 through channel 100.49 every 0.01 channel.

The choice of the ranges for N and s is based on statistics considerations : For example, 100 counts in the MPC of a peak are poor statistics while the accuracy will not change much when increasing the number of counts in the MPC beyond 10 000 counts.

Channel number 100 has been arbitrarily chosen to serve as the center channel for the distributions. Half a channel as the range for the mean suffices to study the full dependence of FWHM on the mean because FWHM changes periodically with the mean, the period being one channel, and because within each channel there is a symmetry in behavior between the first half and the second half of the channel.

3. METHODS OF CALCULATIONS

The methods defined below were used to calculate the FWHM of each of the Gaussians generated :

Methods F1 : This method relies on the definitic of FWHM.

Find the MPC of the peak and N, the number counts in that channel, find the first channel on th right and on the left (c_r , c_l) of the MPC whos counts are less than N/2, linearly interpolate th counts between channel c_l and channel c_{l+1} to fin the channel C_L (fractional) for which the counts a N/2, do the same for channels c_r and c_{r-1} to find C_F calculate FWHM (F1) , / 1 /:

$$\text{FWHM (F1)} = C_R - C_L$$

Method F2 : The method uses the relation betwee the definite integral of a Gaussian, its variance ar its amplitude, / 4 /, calculate the total number counts of the peak (T), find N, calculate FWHI (F2) :

$$\text{FWHM (F2)} = (8 \ln 2/2p)^{1/2}\ T/N$$

Mehod F3 : This method relies on th second-moment calculation of a distribution, and th identity of that moment and s for a Gaussian :

Compute T and the two sums :

$$T_1 = \Sigma\ i\ G(i),$$

$$T_2 = \Sigma\ i^2\ G(i),$$

Over all the channels i of the Gaussian G, calculat the measured mean m_m, the measured standar deviation σ_m and FWHM(F_3), / 5 / :

$$\mu_m = T_1 / T$$

$$\sigma_m = (T_r/T - \mu_m{}^2)^{1/2}$$

$$\text{FWHM(F3)} = (8 \ln 2)^{1/2}\ \sigma_m$$

Method F4 : Uses the least-squares method to f the Gaussian to a parabola often taking the natura logarithm of the Gaussian values.

The function P to which the Gaussian, after takin the natural logarithm is to be fitted is, / 3 / :

$$P = a\, i^2 + b\, i + c,$$

i being the channel number. The parabol

coefficients are related to the Gaussian parameters by the following relations :

$$\sigma_{m2} = -1/(2a)$$

$$\mu_m = -b/(2a)$$

$$\ln(N_m) = c - b^2/(4a)$$

4. RESULTS AND DISCUSSION

The dependence of the relative error in the calculated FWHM on the parameters of the smooth Gaussians (G_2) is shown in Figures (1-6). The relative error r (in percent) is defined as, / 4 / :

$$r = 100\,(FWHM_m / (8 \ln 2)^{1/2} - \sigma) / \sigma$$

Where σ is the true standard deviation of the G_2 Gaussian, and $FWHM_m$ is the result of calculating the FWHM value by each of the four methods.

Generally, for all the methods, the relative error decreases with increasing N. With methods F1 and F2 r exhibits a monotonous dependence on the true mean, this dependence decreases with increasing s and with decreasing N. Also the relative error with these methods is mostly positive, i.e., the calculated FWHM value is larger than its true value.
Method F4 shows a non regular behavior, with sharp changes in the relative error as a function of the true mean. Also, the relative error is mostly negative, which means that the calculated FWHM is smaller than its true value.

Of all methods, F3 exhibits the least sensitivity to all the parameters discussed.

The results for the randomly generated Gaussians (G_1) are presented in this way : For each of the values of s and N the relative error in FWHM fr50 Gaussians with different true μ's are grouped together and the average relative error (r_{av}) and standard deviation (S) about that average are calculated and shown in Figs 7-10 . This way of presentation is used to average out the different fluctuations appeared among different Gaussians.

Comparison among these figures shows that r_{av} is always positive and the smallest values are achieved by F3. The third method has also the least s and the least sensitivity of σ and r_{av} to s, this is the most accurate method.

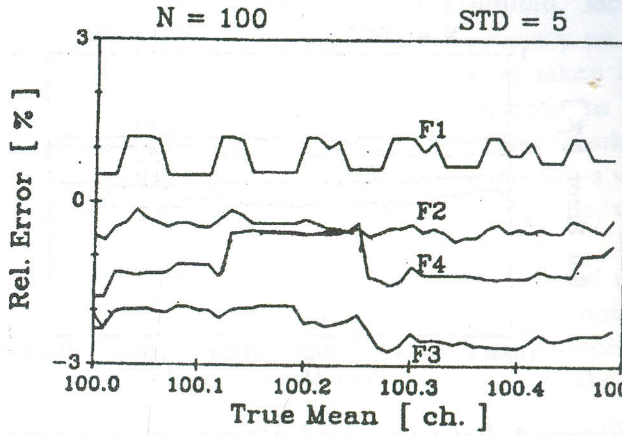

Figure 1. Relative error Vs true mean for a smooth (G_2) Gaussian with N = 100 and σ = 5.

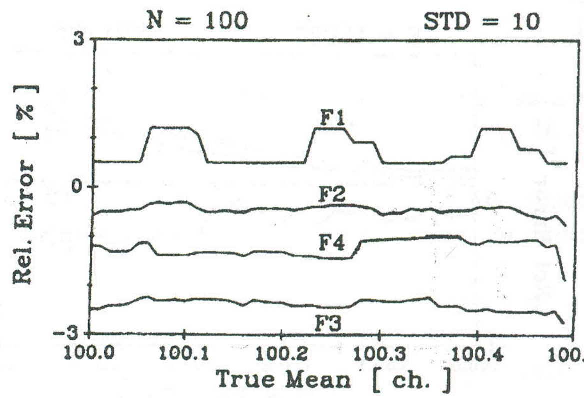

Figure 2. Relative error Vs true mean for a smooth (G_2) Gaussian with N = 100 and σ = 10.

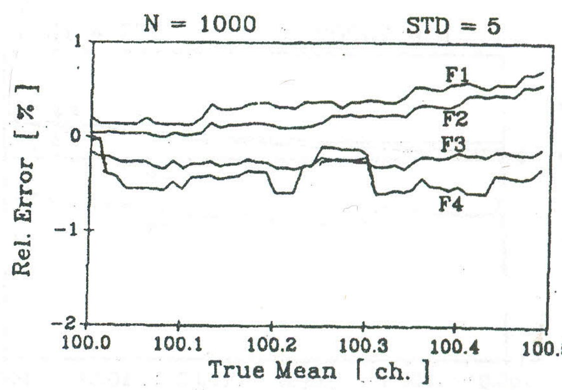

Figure 3. Relative error Vs true mean for a smooth (G_2) Gaussian with N = 100 and σ = 5.

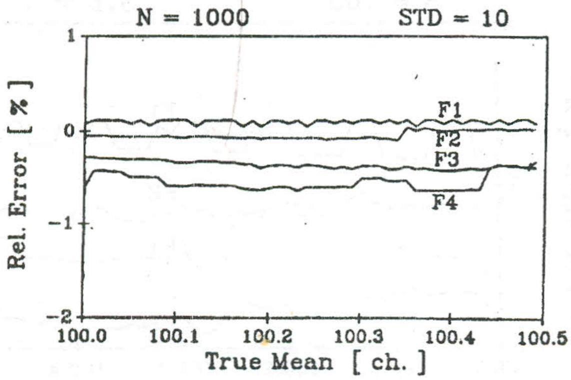

Figure 4. Relative error Vs true mean for a smooth (G_2) Gaussian with N = 1000 and σ = 10.

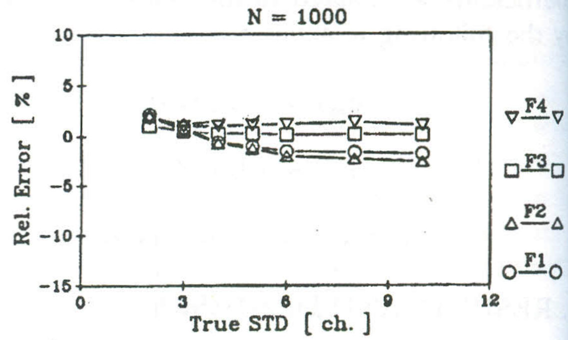

Figure 7. Average relative error Vs true σ for random (G_1) Gaussians with N = 1000.

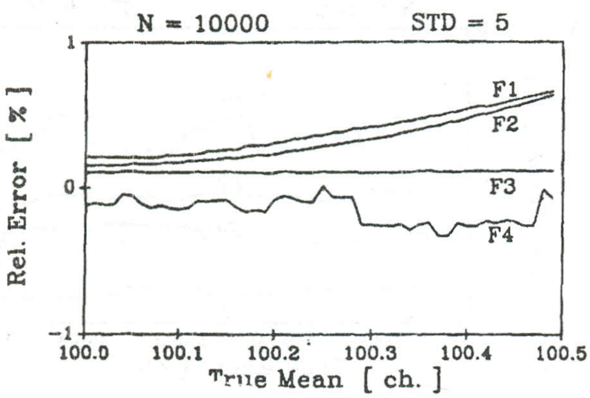

Figure 5. Relative error Vs true mean for a smooth (G_2) Gaussian with N = 10000 and σ = 5.

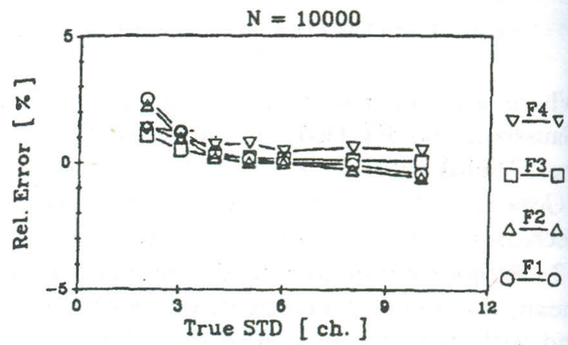

Figure 8. Average relative error Vs true σ for random (G_1) Gaussians with N = 10000.

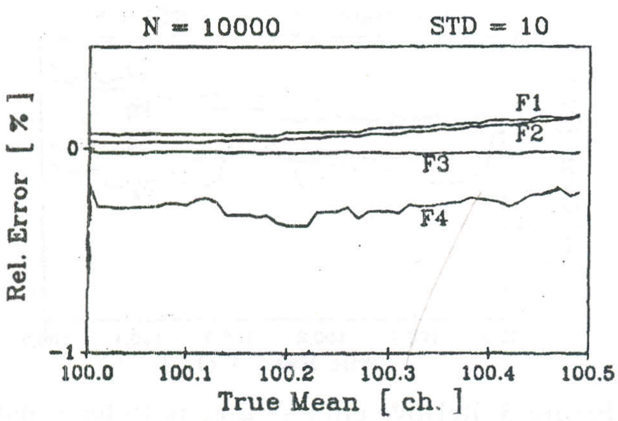

Figure 6. Relative error Vs true mean for a smooth (G_2) Gaussian with N = 10000 and σ = 10.

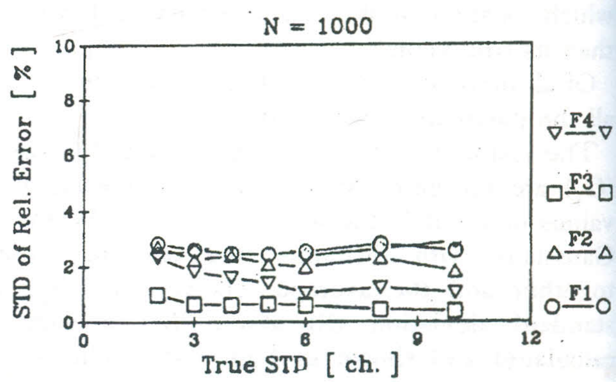

Figure 9. Standard deviation about the average relative error V_s true σ for 50 random (G_1) Gaussians with N =10000.

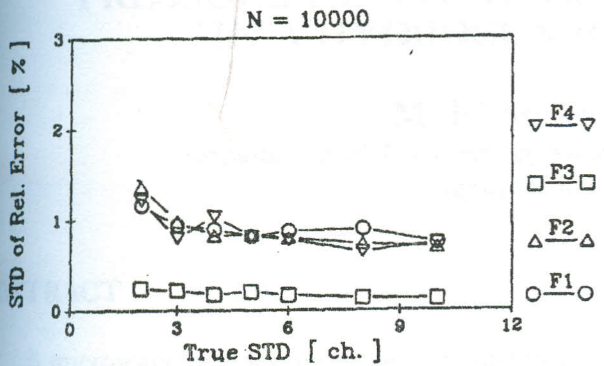

Figure 10. Standard deviation about the average relative error V_s true σ for 50 random (G_1) Gaussians, with N =10000.

5. CONCLUSIONS

All four methods for calculating FWHM discussed in this paper yield accuracies of 10 % or better depending on the distribution parameters.

In applications where this degree of accuracy is sufficient, each one of these methods can be used.

When better accuracy is desired, the recommended method is F3, the second moment of the peak method which is the most accurate of all methods discussed.

When computing resources are limited, factors concerning the dependence of the accuracy on the parameters of the distribution must be taken into account before selecting the method to be employed. If in an application a constant "working point" in terms of N and s can be maintained, a very low error in FWHM can be achieved even with methods F1 and F2.

When the measurement system is to be used with distributions of diverse characteristics, the method that exhibits the least dependence on the parameters of the distributions should be employed, the F3 method.

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