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STATISTICAL EVALUATION AND MEASURING STRATEGY
FOR EXTREMELY SMALL LINE SHIFTS

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ABSTRACT

For a measuring situation limited by counting statistics, but where the level of precision is such that possible systematic errors are a major concern, it is proposed to determine the position of a spectral line from a measured line segment by applying a bias correction to the centre of gravity of the segment. This procedure is statistically highly efficient and not sensitive to small errors in assumptions about the line shape. The counting strategy for an instrument that takes data point by point is also considered. It is shown that an optimum ("two-point") strategy exists; a scan of the central part of the line is 68% efficient by this standard.

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List of symbols

a	range parameter (Fig. 1). Full range of scan is $2a$.
b, B	width of square wave response function (Appendix 2). $b = B/\Gamma$.
c	intensity of second component of line (Appendix 1).
f	bias correction [Eq. (1)].
$I(x)$	line profile.
i	index of measuring point (Section 3.2).
M_0, M_1	zeroth and first central moment of the line segment (Sections 3.1 and 3.2).
n_i	number of counts at point i (Section 3.2).
R_0	peak counting rate of line.
R_i	counting rate at setting i .
s	dimensionless range parameter $s = 2a/\Gamma$.
T	total counting time (Section 3.2).
t	dummy variable (Section 3.2).
x	position variable (Fig. 1).
$\pm x_M$	position settings in two-point strategy (Section 4.2).
z	centre of gravity, $z = M_1/M_0$ (Section 3.2).
α	reduced variance (Fig. 2, Section 5).
Γ	full width at half maximum for Breit-Wigner or Gaussian line.
$\delta(x - x_M)$	Dirac δ function [Eq. (11)].
Δ	position of line (Fig. 1).
ε	energy of second component of line (Appendix 1).
ν	number of measuring points per unit distance of scan.
$\tau, \tau(x)$	counting time per point.

1. INTRODUCTION

In recent experiments^{1,2)} we determined shifts in the energies of K X-rays to a precision better than one thousandth of the natural line width. Although the principal limitation was counting statistics, it was clearly also important to pay great attention to possible sources of systematic errors, and it was in particular felt that normal curve-fitting techniques were potentially unsafe. Errors could come about not only as a result of systematic deviations between the true and the assumed line shape, but also because of the existence (demonstrated in Ref. 2) of variations in the true shape from one line to another. In the present paper is described a statistical method which is i) essentially as efficient as a least squares adjustment, ii) simple to use, and iii) insensitive to small variations in the line shape. The discussion of the efficiency of the statistical evaluation furthermore leads to a general discussion of the efficiency of the strategy of data-taking.

Although the treatment given in the following is oriented towards a particular type of application in experimental physics, it is important to realize that the problem has much in common with one of the classical objectives in the statistical theory of estimation³⁾, that of determining the location parameter for a statistical variable. Hence a brief discussion of this problem is useful and also serves to define some of the statistical terminology used in the present work. Let a statistical variable v be distributed with probability density $p(v)$. From a series of observations $v_1, v_2, \dots, v_N$ we now try to derive estimates (often called measured values) of the parameters characterizing $p(v)$. We are especially interested in a precise estimate of the location parameter, which gives the position of the curve $p(v)$, while for our purpose it is sufficient to have approximate values for other parameters. A mathematical procedure for deriving an estimate from the set $v_1, v_2, \dots, v_N$ is called an estimator, of which common examples are mean, median, mode, etc.

Each estimator will lead to a particular variance on the estimate, and normally preference will be given to the one that gives the smallest value. It is therefore important that it is possible to derive a lower limit^{3,4)} on the variance

("minimum-variance bound", "Cramér-Rao inequality") relative to which the efficiency of an estimator may be defined. There often will exist a minimum-variance estimator, as, for example, the mean for a normal distribution. A special though not uncommon problem occurs if the function $p(v)$ is poorly known. In this case we are led to consider estimators that are insensitive to the details of $p(v)$; this is known as "robust" or "distribution-free" estimation³⁾, and involves effectively a trade-off between safety and efficiency, where a "safe" procedure is one that minimizes the error for the worst thinkable situation.

The spectroscopic problem, in which N counts have been obtained in a scan across a line profile $I(x)$, is formally identical to N observations of the statistical variable x_i , provided that the scan is infinitely wide. The arbitrary choice of the beginning and end of the scan, however, distorts the "sample", and necessitates what in statistical language is called a "bias correction". Because of the bias correction, the minimum-variance bound will be higher in the spectroscopy case than in the sampling case. The results for the spectroscopic problem presented in the following are thought to be applicable to a wide class of experiments, and they are therefore given in a general form. The specific application underlying the present work will be described in detail elsewhere⁵⁾.

2. FORMULATION OF THE PROBLEM

Let the spectrometer record the counting rates R_i at consecutive settings x_i . The problem is now to derive an estimate of the location parameter Δ from the set of data x_i, R_i . It may be useful to think of Δ as the mid-point of a symmetric line, but it is really only essential to have a consistent definition allowing a comparison with a reference line, measured or calculated. Thus, although our treatment discusses the location parameter of one line only, any real experiment involves a comparison of two lines, as may be seen from three examples:

- i) A reference line of the same shape is superimposed. At the setting i two intensities R_i^I and R_i^{II} are recorded, so that if the overlap is ideal the errors in the spectrometer settings will become negligible. The shift is then simply $\Delta^I - \Delta^{II}$, as in our experiments^{1,2,5)}.

- ii) The line and its reference cannot be brought to overlap, and also the errors in the x_i must be taken into account explicitly.
- iii) Absolute measurement. There is no reference line, and errors in the theoretical line shape, errors in the settings x_i , and counting statistics must all be taken into account.

Two main types of lines are of interest in the present work: the Gaussian $I(x) = \exp(-4x^2 \ln 2/\Gamma^2)$, and the Breit-Wigner shape $I(x) = (1 + 4x^2/\Gamma^2)^{-1}$, the latter known to statisticians as the Cauchy distribution. Shapes representing a folding of the two have been discussed by Wilkinson⁶⁾; a simple correction for the spectrometer resolution is discussed in Appendix 2.

The treatment given in the following incorporates explicitly only the errors arising from counting statistics*). Starting from an arbitrary but intuitively attractive measuring strategy and data treatment, we try to answer four questions:

- 1) What is the unbiased estimate of the location parameter?
- 2) What is the resulting error, and how can the counting time best be distributed?
- 3) What is the statistical efficiency of the method of estimation?
- 4) Is there an optimum strategy for the data-taking and how efficient is our method relative to that?

3. THE CENTRE OF GRAVITY OF A TRUNCATED LINE

It is intuitively evident that the data-taking should be concentrated around the central part of the line; we now consider an especially simple strategy consisting in scanning the line with constant counting time per unit interval. The method and notation is summarized in Fig. 1. It is assumed that the scan starts at a point $-a$ below the expected location and ends at $+a$ above, and we now attempt to derive an estimate of the true line position Δ from the truncated line. This procedure is similar to the trimming³⁾ used for infinite samples, but it is evident that the centre of gravity of the truncated line does not represent a correct estimate of Δ .

*) In particular, the contribution from the background can be left out, as the very high precision envisaged here cannot be attained if the background plays a major role.

3.1 The bias correction

We expand the line shape as a Taylor series in Δ :

$$I(x - \Delta) \cong I(x) - \Delta I'(x) + \frac{1}{2} \Delta^2 I''(x) - \dots$$

By exploiting the symmetry properties of $I(x)$ (Fig. 1), we find for the zeroth moment of the line

$$M_0 \cong R_0 \tau \nu \int_{-a}^a I(x) dx + \text{term in } \Delta^2,$$

and similarly through integration by parts for the first moment,

$$M_1 \cong R_0 \tau \nu \Delta \left[\int_{-a}^a I(x) dx - 2aI(a) \right] + \text{term in } \Delta^3.$$

Consequently an unbiased first-order estimate of the location parameter is

$$\Delta = \frac{M_1}{f M_0}, \quad (1a)$$

with

$$f = 1 - 2aI(a) \left/ \int_{-a}^a I(x) dx \right., \quad (1b)$$

plus higher terms. Note that the line shape $I(x)$ enters only in the scale correction f , and that the centre of gravity $z = M_1/M_0$ is distribution-free. It is in fact possible and sometimes convenient to determine the parameter f empirically from the convergence of an iterative procedure. The f values used in previous work^{1,2)} have usually been accurate to 2-5%.

3.2 The variance on Δ

Let the scan from $-a$ to a be carried out in $2a\nu + 1$ steps corresponding to a total measuring time $T = (2a\nu + 1)\tau$. Numbering*) the steps from $i_{\min} = -a\nu$ to $i_{\max} = a\nu$, we have

$$M_0 = \sum_i n_i \quad \text{and} \quad M_1 = \sum_i n_i (i\nu^{-1}),$$

with errors from counting statistics determined by the Poisson law,

$$\text{var } n_i \cong n_i,$$

valid for large n_i . In this limit the variance of Δ may be expressed:

*) To simplify the notations, it is assumed that $a\nu$ is an integer. A realistic calculation must take the (trivial) end-point corrections into account.

$$\text{Var } \Delta = f^{-2} \text{Var } z \cong f^{-2} \sum_{-av}^{av} \left(\frac{\partial z}{\partial n_i} \right)^2 \text{Var } n_i \cong \frac{1}{R_0 T} \frac{2a \int_{-a}^a x^2 I(x) dx}{\left[\int_{-a}^a I(x) dx - 2aI(a) \right]^2}, \quad (2)$$

where the n_i have been approximated by their true values.

3.3 Results for specific line shapes

Let the line shape be expressed in terms of the full width Γ at half maximum, and introduce the range parameter $s = 2a/\Gamma$. From Eqs. (1) and (2) we now obtain for a Breit-Wigner line shape

$$f_{BW} = 1 - \frac{s}{(1 + s^2) \arctan s} \quad (3)$$

$$\text{Var } \Delta_{BW} = \frac{\Gamma^2}{R_0 T} \frac{s(s - \arctan s)}{\left[2 \arctan s - \frac{2s}{1 + s^2} \right]^2}, \quad (4)$$

and for a Gaussian line shape

$$f_G = 1 - \frac{2(\ln 2)^{1/2} s \exp(-s^2 \ln 2)}{\pi^{1/2} \Phi[s(\ln 2)^{1/2}]}, \quad (5)$$

$$\text{Var } \Delta_G = \frac{\Gamma^2}{4(\pi \ln 2)^{1/2} R_0 T} \left\{ \frac{1}{s} \Phi[s(\ln 2)^{1/2}] - 2 \left(\frac{\ln 2}{\pi} \right)^{1/2} \exp(-s^2 \ln 2) \right\}^{-1} \quad (6)$$

where the definition of the probability integral is

$$\Phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt.$$

The functions $\text{Var } \Delta$ are shown in Fig. 2, from which it can be seen that for a given measuring time there exists an optimum for the range parameter $s = 2a/\Gamma$. For the case of a Breit-Wigner shape, the optimum occurs for $s \cong 1.1$ and leads to $\text{Var } \Delta_{BW} = 0.64 \Gamma^2/R_0 T$, while for a Gaussian shape it occurs for $s \cong 2$ corresponding to $\text{Var } \Delta_G = 0.36 \Gamma^2/R_0 T$. An approximation to a mixed shape is discussed in Appendix 2.

It is clearly possible to define many other estimators than the one defined in Eq. (1). We have investigated the bias-corrected median of the truncated line, but find for $s \leq 2$ that the centre-of-gravity method always remains the best choice.

In short, then, our recommended procedure is to scan the line only in the optimum interval and to estimate the location parameter from Eq. (1). The statistical error on the estimate is given by Eq. (2). We now examine to what extent it is possible to do better.

4. THE EFFICIENCY OF THE METHOD

In analogy with common usage in statistics⁵⁾, we define the efficiency of a given (experimental and statistical) procedure as proportional to the reciprocal of the time required to reach a given variance on the position estimate for fixed line shape and source strength. By deriving the minimum variance, it becomes possible to express the efficiency on an absolute scale. In the following we consider first the statistical efficiency of the procedure of Section 3; following this, we derive an optimum strategy.

4.1 The matching of line profiles

Müller et al.⁷⁾ have obtained an expression for the precision with which a known line profile $I(x)$ can be fitted to a measured scan of the line so that a least squares fit is obtained. Let the number of counts at position x_i be n_i ; the difference between n_i and the true value $R_0 \tau I(x_i)$, which we here assume known, then provides one estimate Δ_i of the line position

$$\Delta_i = [R_0 \tau I(x_i) - n_i] \left[R_0 \tau \left(\frac{dI(x)}{dx} \right)_{x_i} \right]^{-1}$$

with variance

$$\text{Var } \Delta_i = \frac{1}{R_0 \tau} \frac{I(x_i)}{\left[dI(x)/dx \right]_{x=x_i}^2},$$

where we have used $\text{var } n_i = R_0 \tau I(x_i)$, valid for $n_i \gg 1$. The resulting shift Δ is obtained as a weighted average over the Δ_i , and the reciprocal variance, which must represent an upper-limit, is expressed by

$$\begin{aligned} [\text{Var } \Delta]_{\text{limit}}^{-1} &= \sum_i [\text{Var } \Delta_i]^{-1} \\ &= R_0 \tau \int_{-a}^a \frac{[dI(x)/dx]^2}{I(x)} dx, \end{aligned} \quad (7)$$

where the last expression replaces the sum over ν points per unit interval by an integral.

Applied to a Breit-Wigner line shape, Eq. (7) yields

$$(\text{Var } \Delta)_{\text{limit}} = \frac{\Gamma^2}{R_0 T} \left[-\frac{4}{(1+s^2)^2} + \frac{2}{(1+s^2)} + \frac{2 \arctan s}{s} \right]^{-1}, \quad (8)$$

where s is the range parameter $s = 2a/\Gamma$. The function $(\text{Var } \Delta)_{\text{limit}}$ is shown in Fig. 2; at the minimum ($s = 1.1$) it attains the value 0.625 for the reduced variance as compared with 0.663 for the method of Section 3, which thus has an efficiency of 96%. For larger values of s , the efficiency clearly becomes poorer (83% for $s = 2$, 69% for $s = 3$); this reflects the well-known fact that the centre of gravity is an estimator of zero efficiency for an infinite Breit-Wigner distribution.

Applied to a Gaussian line shape, the expression (7) directly gives back the expression (6) so that our procedure in this case is 100% efficient for all values of s . It is easy to see why this is so as the proof^{4b)} that the centre of gravity is a minimum-variance estimator for a normal distribution applies also to a truncated normal distribution.

4.2 The efficiency of the data-taking strategy

Until now, we have considered a strategy consisting in equal counting time per point (density of points ν) for an interval $-a$ to a . The best choice is to take $a = 0.55 \Gamma$. We now allow the counting time to be a function $\tau(x)$ of the position x . The total counting time is

$$T = \nu \int_{-\infty}^{\infty} \tau(x) dx. \quad (9)$$

From the method of matching of line profiles discussed above, the expression for the reciprocal of the limiting variance can be arrived at:

$$[\text{Var } \Delta]_{\text{limit}}^{-1} = R_0 \nu \int_{-\infty}^{\infty} \frac{\tau(x) [dI(x)/dx]^2}{I(x)} dx, \quad (10)$$

which we wish to maximize subject to the constraint (9). The solution is evidently

$$\tau(x) = \frac{T}{\nu} \delta(x - x_M), \quad (11)$$

where $\pm x_M$ are the values of x that maximize $[dI(x)/dx]^2/I(x)$, so that we have

$$[\text{Var } \Delta]_{\text{limit}}^{-1} = R_0 T \left[\frac{[dI(x)/dx]^2}{I(x)} \right]_{|x|=x_M}, \quad (12)$$

which corresponds to a limit for an optimized "one-point" strategy. A practical version of this strategy is to measure equal times τ at $-x_M$ and at $+x_M$ giving n_- and n_+ counts. The true line position may then be obtained from

$$\Delta = \frac{n_+ - n_-}{2R_0\tau |dI(x)/dx|_{x=x_M}}, \quad (13)$$

where the peak counting rate R_0 is best determined from a short measurement at $x = 0$. This strategy allows the limit (12) to be attained.

For a Breit-Wigner line shape we find $x_M = \pm 8^{-1/2}\Gamma$ and

$$[\text{Var } \Delta]_{\text{limit}}^{\text{B-W}} = 0.422 \frac{\Gamma^2}{R_0 T},$$

showing that the strategy of Section 3 (equal counting time per unit interval, $s = 1.1$) is 68% efficient. Likewise for a Gaussian line shape we have

$$x_M = \pm 2^{-1}(\ln 2)^{-1/2}\Gamma \text{ and}$$

$$[\text{Var } \Delta]_{\text{limit}}^{\text{G}} = 0.245 \frac{\Gamma^2}{R_0 T},$$

showing that the strategy of Section 3 (equal counting time per unit interval, $s = 2$) is 67% efficient.

5. CONCLUDING REMARKS

The present work is oriented towards a situation where one wishes to determine the position Δ of a line with very high precision, typically 10^{-3} of the line width, expressed as the full width Γ at half maximum. A convenient figure of merit is α^{-1} given by $\text{Var } \Delta = \alpha\Gamma^2/R_0T$, where R_0 is the peak counting rate and T is the total time allotted to the measurement. The main conclusions are the following:

A) For a spectrometer that takes data point by point, there exists an optimum counting strategy, which consists in counting essentially only the wings of the line [Eqs. (10)-(13)], and which leads to $\alpha = 0.42$ (Breit-Wigner line shape). This strategy, although clearly a realistic one, is considered to be too vulnerable to systematic errors; instead we prefer the one given in Section 3. The preferred strategy scans uniformly across a truncated line and is 68% efficient (in statistical terms) relative to the optimum strategy.

B) For the case of the truncated line we develop a robust (or distribution-free) method of estimation based on the centre of gravity with a bias correction [Eq. (1)]. It is shown that the statistical efficiency of this method is close to 100%.

The concepts developed here should have many applications. It is probably worth underlining that the use of a distribution-free approach has allowed us to discuss²⁾ in a well-defined way the differences in position of lines with different shapes.

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THE PROPERTIES OF A COMPOSITE BREIT-WIGNER LINE

The results given in Section 3 have assumed a symmetrical line shape. It is easily seen that the presence of a small asymmetry will appear as a constant shift in the energy. We take here as an example a Breit-Wigner line made up of two components, one at energy zero and with intensity $1 - c$, and another at energy ϵ and with intensity c . For $\epsilon \ll \Gamma$ it is found that the peak location is $\Delta = \epsilon c +$ terms in ϵ^3 . The full width at half maximum becomes

$$\text{FWHM} = \Gamma + \frac{5\epsilon^2}{\Gamma} c(1 - c) ,$$

so that the branching is quadratic in ϵ/Γ , while an asymmetry will show up only in the cubic terms.

A BREIT-WIGNER VIEWED THROUGH A SQUARE WAVE

The experimental line profile will be intermediate between the natural shape (a Breit-Wigner curve) and the instrumental resolution function, often similar to a Gaussian. The case of a Breit-Wigner viewed through a Gaussian has been discussed by Wilkinson⁶⁾; here we give some results for the simple case where the resolution function is approximated by a square wave of width B, or, in dimensionless units $b = B/\Gamma$. The folded line is

$$I(E) = \frac{1}{2} b^{-1} \left[\arctan\left(\frac{2x}{\Gamma} + b\right) - \arctan\left(\frac{2x}{\Gamma} - b\right) \right], \quad (A2.1)$$

with full width at half maximum

$$FWHM = (\Gamma^2 + B)^{1/2} = \Gamma(1 + b^2)^{1/2}.$$

The maximum value is

$$I_0 = \arctan b/b$$

and the bias correction [Eq. (1b)]

$$\begin{aligned} f = 1 - s & \left[\arctan(s + b) - \arctan(s - b) \right] \\ & \left[(s + b) \arctan(s + b) - (s - b) \arctan(s - b) \right. \\ & \left. + \frac{1}{2} \ln \frac{1 + (s - b)^2}{1 + (s + b)^2} \right]^{-1}. \end{aligned} \quad (A2.2)$$

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Figure captions

- Fig. 1 : The truncation procedure. The profile of the line is given by $R(x) = R_0 I(x - \Delta)$, where R_0 is the peak counting rate and $I(x)$ the symmetric shape. The origin of the coordinate system is chosen to correspond to the assumed location of the line, and Δ represents the true location parameter. The line is scanned from $-a$ to a at equal intervals and at equal counting time per point.
- Fig. 2 : Standardized variance [i.e. in units of $\Gamma^2/(R_0 T)$] as a function of counting strategy for the centre-of-gravity method. The parameter s is the range scanned expressed in units of the half width Γ , R_0 is the peak counting rate, and T is the total counting time. The results are shown for a pure Breit-Wigner shape and for a pure Gaussian shape. The dashed curve indicates the theoretical minimum-variance limit for a Breit-Wigner shape.

Fig. 1

Fig. 2