be neglected and the familiar formula for short-range-order diffuse scattering (see *e.g.* Guinier, 1963, p. 269) is obtained. For values of σ much greater than this many such diffuse curves corresponding to higher values of P must be included in the summation. Each of these will represent successively broader more diffuse peaks as r^{2P} approaches zero. The factor $(k^2\sigma^2)^P/P!$ eventually goes to zero as P increases for any σ but for values of $\sigma \simeq 1$ many terms must be included.

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Relationship between 'Observed' and 'True' Intensity: Effect of Various Counting Modes

BY A. J. C. WILSON

Department of Physics, University of Birmingham, Birmingham B15 2TT, England

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Abstract

Expressions for the probability $p(R_o)$ that a reflexion of 'true' intensity R will have an observed value R_o (possibly negative) are obtained for four counting modes: fixed-time counting, equal and unequal times for total and background; fixed-count timing, equal and unequal counts for total and background. The distributions have a positive excess and are in general skew, though the skewness may be zero for particular choices of unequal times (counts). Deviations from the normal distribution with the same mean and variance may be considerable for $|R_o| \simeq 0$ and for $|R_o|$ large, and may possibly be significant in some applications even for $R_o \simeq R$. This apparent conflict with the central limit theorem is reconciled.

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1. Introduction

In both single-crystal and powder diffractometry the integrated intensity of a reflexion is obtained as the difference between a counting rate averaged over a region of reciprocal space intended to include the reflected intensity, and a counting rate averaged over a neighbouring volume of reciprocal space intended to include only background. If the intentions are not effectively realized there will be a systematic error in the measured intensity, but the present concern is not with such systematic errors but with statistical fluctuations in the intensity as observed. Although an intensity can never be really negative, it is not uncommon for the measured background counting rate to be higher than the measured reflexion-plus-background rate, giving an observed-as-negative reflexion. The probability of an observed-as-negative intensity will depend on the counting mode in which the diffractometer is operated.

The two basic modes (Parrish, 1956) are fixed-time counting and fixed-count timing. In the first, each measurement is made in a pre-determined time interval, and the standard deviation of the observed counting rate is proportional to the square root of the true (mean) counting rate. In fixed-count timing the counting is continued until a pre-determined number of counts is reached, and the standard deviation of the observed counting rate is proportional to the true counting rate. In other words, the relative error in intensities goes down inversely as the square root of the intensity for fixed-time counting, whereas the relative error is independent of the counting rate in fixed-count timing. Each method has advantages, depending on the purpose of the measurements, and numerous modifications and compromises have been used in practice or proposed with the object of increasing the efficiency of the use of the available time. Among these are:

(i) The Cooke-Yarborough (1951) method. Fixed-count timing suffers from the disadvantage that the diffractometer spends most of its time accumulating background counts at a low rate, and much less on the reflexion. This is avoided if artificial counts are fed into the counting circuits at a known uniform rate. The diffractometer mode thus approximates to fixed-count timing while on a reflexion where the counting rate is already high, and to fixed-time counting while on the background where the counting rate is low. This method has advantages in some applications of powder diffractometry, but I have not come across any mention of its use in single-crystal diffractometry.

(ii) Multiple fixed-time counting. The diffractometer control circuits are arranged so that counts are accumulated for a predetermined unit of time. If the number is great enough to give a satisfactorily low expected standard deviation the diffractometer moves on to the next measurement. If the number is not great enough the measurement is repeated for a further time unit, and the pooled number of counts tested, the process being repeated until *either* a satisfactory standard deviation is achieved, *or* a predetermined number (say five to twenty) of time units has been used. Like the Cooke-Yarborough method, this approximates to fixed-count timing where counting rates are high, and to fixed-time counting where they are low. It is described in detail by Mackie (1972) and briefly by Sudarsanan & Young (1974).

(iii) Optimization of counting times. Procedures for optimizing counting times for the achievement of different purposes have been proposed by many authors, but it seems that they have usually been proposals never realized routinely. The following are some typical papers, in order of date: Mack & Spielberg (1958), Zevin, Umanskij, Khejker & Pančenko (1961), Wilson, Thomsen & Yap (1965), Killean (1967), Wilson (1967), Shoemaker (1968), Thomsen & Yap (1968*a*,*b*), Shoemaker & Hamilton (1972), Mackenzie & Williams (1973), Killean (1973), Grant (1973) and Szabó (1978).

The determination of the probability distribution of the measured intensity of a reflexion is of intrinsic intellectual interest. There are, however, three possible applications of practical interest in structure determination. First, French & Wilson (1978) have proposed a Bayesian method of estimating a more likely positive value for the intensity of a reflexion actually measured as negative. The method requires a knowledge of the probability distribution of measured-as-negative intensities. Their assumption that the distribution is the tail of a normal distribution is not entirely accurate; substitution of a more accurate distribution would not affect the principle of the method, though it would alter the actual values obtained. French (1978) and one of the referees of this paper estimated the bias that would result from using the normal approximation rather than the 'true' distributions in the French & Wilson (1978) procedure; the estimates range from 1 to 10% in the likely range of application. Although this amount is not large, it is a systematic bias rather than a random error, and would thus bias estimates of crystallographic parameters (Wilson, 1973, 1976, 1979). Outside the likely range of this application the relative error becomes larger, and may be of importance in other applications.

Secondly, Price (1979) has proposed a maximum-likelihood method of estimating structural parameters, as an improvement on the usual procedures. This method requires a knowledge of the probability distribution of the measured intensities; maximum-likelihood and least-squares estimates coincide only if the intensity distribution is normal with known variance. The exact distribution near the peak is thus of interest for the Price procedure; Price actually assumed a Poisson distribution, which in some senses differs from the normal more than the 'true' distribution does (Table 1). All the 'true' distributions considered here have a positive excess (kurtosis), as does the Poisson; this implies that they are slimmer near the peak and have more pronounced tails than the normal distribution (Cramér, 1945, p. 184). To be more specific, if a distribution differed from the normal only through having a finite positive excess, it would lie above the normal in the range $\pm 0{\cdot}742$ standard deviations, below it in the ranges $\pm(0{\cdot}742,\ 2{\cdot}332)$, and above it again in the ranges $\pm(2{\cdot}332,\ \infty)$. The distributions to be considered are in general skew, though the skewness may vanish for particular values of the ratio of counting times or of timing counts (Table 1).

The third way in which a knowledge of the probability distribution of measured intensities could be of practical use is in the indication of structural imperfection or systematic error. Certain types of structural imperfection give a displacement as well as a broadening of the reflexions, the displacement varying systematically with *hkl*. If this is not recognized, routine diffractometer measurements would find background at the position of the undisplaced reflexion and reflexion or part of a reflexion at the 'background' setting, giving a measured-as-negative reflexion corresponding to a physical reality. There is also the possibility that a rapidly varying thermal or other diffuse background may be higher at the background setting than at the reflexion setting, giving a measured-as-negative reflexion instead of a weak positive reflexion. Finally, there is the possibility that at extreme settings more stray radiation may reach the detector when on background than when on a reflexion, though this is not likely to happen systematically. If the proportion of measured-as-negative reflexions is greatly in excess of that to be expected from the relevant probability distribution, a photographic check on displacement of reflexions or abnormal background may be worth while.

It may avoid confusion to point out that intensities have two distinct probability distributions: the *a priori* probability that an arbitrarily chosen reflexion of a particular substance will have a particular 'true' intensity (R in the notation of the present paper) (Wilson, 1949), and the probability that a 'true' R will have an observed value R_o. It is the second type of probability distribution that is now under discussion, but both are needed for the French & Wilson (1978) procedure. The complexity of the mathematics increases rapidly with the complexity of the counting mode, and only four possibilities are considered here:

(i) fixed-time counting with equal background and total times;

(ii) fixed-time counting with different background and total times;

(iii) fixed-count timing with equal background and total counts; and

(iv) fixed-count timing with different background and total counts.

Results in terms of familiar functions are obtained only for the first of these (§2). The second requires a recognized but not familiar function (§3); for the third and fourth only a series valid for small values of R_o is obtained (§4). This is, however, sufficient for a discussion of the applicability of the normal approximation in the French & Wilson (1978) procedure. Often the probability of small positive or small measured-as-negative reflexions is less than that predicted by the normal approximation. The relative discrepancies can be large for $|R_o|$ near zero and for $|R_o|$ large, so a reconciliation with the central limit theorem (asymptotic approach to normality of probability distributions satisfying certain requirements) is attempted in §5.

2. Fixed-time counting

In the absence of drift and other disturbing influences (such as the use of unrectified or unsmoothed high-tension supplies for the X-ray tube), the number of photons recorded during the predetermined time interval used in diffractometers working in the fixed-time mode will fluctuate in accordance with the Poisson probability distribution. If the 'true' number of counts to be expected in the interval is N, the probability that the observed number will be N_o is given by

$$p(N_o) = \exp(-N)N^{N_o}/N_o!, \qquad (1)$$

Table 1. *Some parameters of the intensity distributions*

Distribution	Mean μ	Variance σ^2	Skewness γ_1	Excess γ_2
Poisson	T	T	$T^{-1/2}$	T^{-1}
Normal	μ	σ^2	0	0
Fixed-time				
equal	$T-B$	$T+B$	$\dfrac{T-B}{(T+B)^{3/2}}$	$\dfrac{1}{T+B}$
unequal	$T-kB$	$T+k^2B$	$\dfrac{T-k^3B}{(T+k^2B)^{3/2}}$	$\dfrac{T+k^4B}{(T+k^2B)^2}$
Fixed-count				
equal	$T-B$	$\dfrac{T^2+B^2}{m-2}$	$\dfrac{4(m-2)^{1/2}(T^3-B^3)}{(m-3)(T^2+B^2)^{3/2}}$	$\dfrac{6(5m-11)(T^2-B^2)}{(m-3)(m-4)(T^2+B^2)}$
unequal	$T-B$	$\dfrac{T^2}{m_1-2}+\dfrac{B^2}{m_2-2}$	Complicated	

where all quantities appearing are necessarily non-negative. If the 'true' number of counts to be expected when the diffractometer is set to receive a reflexion is T, and the 'true' number when it is set to receive the immediate background is B, the 'true' intensity of the reflexion is

$$R = T - B, \tag{2}$$

provided that the time interval used for reflexion is equal to the time interval used for background. In practice, the 'observed' values T_o and B_o fluctuate with probabilities given by (1) with T or B replacing N, so that the observed value,

$$R_o = T_o - B_o, \tag{3}$$

will also fluctuate, though not with the same probability distribution, and can, at times, be observed as negative. The probability of obtaining any particular value of R_o is given by

$$p(R_o) = \sum \exp\{-(B+T)\} B^{B_o} T^{T_o} / B_o! T_o!, \tag{4}$$

the summation being over all values of T_o and B_o satisfying (3). It has already been shown [Wilson (1978), using results of Skellam (1946)] that this summation gives

$$p(R_o) = \exp\{-(B+T)\}(T/B)^{R_o/2} I_{|R_o|}\{2(BT)^{1/2}\}, \tag{5}$$

where I_n is the hyperbolic Bessel function of the first kind. The expression is valid for both positive and negative values of R_o. Obviously

$$p(+|R_o|)/p(-|R_o|) = (T/B)^{|R_o|}, \tag{6}$$

a remarkably simple relationship. Equation (6) suggests that the maximum of $p(R_o)$ near $R_o = R$ will have a miniature counterpart, diminished by the factor $(T/B)^{|R_o|}$ near $R_o = -R$, but in fact the probability falls off so rapidly for negative values of R_o that no miniature peak is achieved.

In view of the possible applications mentioned in the *Introduction* it is of interest to compare the distribution (5) with the normal approximation frequently assumed. This is

$$p(R_o) = (2\pi S)^{-1/2} \exp\{-(R_o - R)^2/2S\}, \tag{7}$$

where S is given by

$$S = B + T \tag{8}$$

and R has the same meaning as before. The comparison is most easily made by expressing the Bessel function as a series asymptotic in $(R_o^2 + 4BT)^{1/2}$:

$$\begin{aligned} p(R_o) \simeq\ & \{4\pi^2(R_o^2 + 4BT)\}^{-1/4} \exp(-S) \\ & \times \{2(BT)^{1/2}/[|R_o| + (R_o^2 + 4BT)^{1/2}]\}^{|R_o|} \\ & \times (T/B)^{R_o/2} \exp\{(R_o^2 + 4BT)^{1/2}\} + \ldots \end{aligned} \tag{9}$$

(Abramowitz & Stegun, 1964, formula 9.7.7). For any reasonable number of counts the terms not written down are quite negligible. There are four comparisons to be made. For R_o large and positive (9) becomes, on neglecting $4BT$ in comparison with R_o^2,

$$p(R_o) \simeq (2\pi R_o)^{-1/2} (T/R_o)^{R_o} \exp(R_o - S), \tag{10}$$

whereas the normal approximation becomes

$$p(R_o) \simeq (2\pi S)^{-1/2} \exp(-R_o^2/2S). \tag{11}$$

Obviously the normal approximation approaches zero much more quickly than the true probability does. At the peak of the normal approximation $R_o = R$, and after considerable cancellation (9) gives

$$p(R) = (2\pi S)^{-1/2}, \tag{12}$$

which is exactly the same as for (7). In other words, the ordinates of the normal approximation and the asymptotic expression for the true probability agree exactly at the peak of the normal approximation. For R_o near zero, the region of interest for the French & Wilson (1978) procedure, (9) becomes

$$p(R_o) \simeq (16\pi^2 BT)^{-1/4} (T/B)^{R_o/2} \exp\{2(B/T)^{1/2} - S\}, \tag{13}$$

which is, in fact, the first term of the usual asymptotic expansion of (5) (Whittaker & Watson, 1935, p. 373; Abramowitz & Stegun, 1964, formula 9.7.1), valid for large values of the variable [in this case $2(BT)^{1/2}$] but not for large values of the order (in this case $|R_o|$). Equation (9) is remarkable for its wide range of applicability for both variable and order. The normal approximation is, of course,

$$p(R_o) = (2\pi S)^{-1/2} \exp(-R^2/2S)\{1 + RR_o/S + \ldots\}, \tag{14}$$

and the relation and the relative magnitudes of (13) and (14) are by no means obvious. However, for assessing the adequacy of the normal approximation for use in the French & Wilson (1978) procedure it will suffice to take the ratio of the probabilities at $R_o = 0$ and, in order to reduce the multiplicitv of symbols, to introduce the total-to-background ratio, say q, so that

$$\begin{aligned} T &= qB, \\ S &= (q+1)B, \\ R &= (q-1)B. \end{aligned} \tag{15}$$

Obviously (in the absence of experimental blunders)

$$q \geq 1. \tag{16}$$

One then has

$$\frac{p(0)\ \text{(Bessel)}}{p(0)\ \text{(normal)}} = \left[\frac{(q+1)^2}{4q}\right]^{1/4} \times \exp\left\{\left[-1 - q + 2\sqrt{q} + \frac{(q-1)^2}{2(q+1)}\right]B\right\}. \tag{17}$$

For $q = 1$ (reflexion of zero intensity), the ratio reduces to unity, in agreement with the identity of (7) and (12), but for increasing q the ratio decreases, particularly if the background is large. The true probability of small positive or negative reflexions is thus less than that suggested by the normal approximation. For large negative reflexions [$|R_o|$ a few times $(BT)^{1/2}$] (9) reduces to

$$p(-|R_o|) \simeq (2\pi|R_o|)^{-1/2}(B/|R_o|)^{|R_o|}\exp(|R_o| - S), \quad (18)$$

and the normal approximation remains as in (11), so that the true probability is once more larger than that given by the normal distribution. Both probabilities are so small that this region is of little interest.

3. Modified fixed-time counting

The simplest modification of fixed-time counting is the use of different counting times for reflexion and background; for example the background may be measured on both sides of the reflexion, over the same time as was used for the reflexion, instead of half the time. The nett number of 'reflexion' counts is then

$$R_o = T_o - \tfrac{1}{2}B_o, \quad (19)$$

where B_o is the total number of background counts, instead of the value given by (3). In general, therefore, the relation between total reflexion-plus-background counts T_o, background-only counts B_o, and reflexion-only counts R_o will be

$$R_o = T_o - kB_o, \quad (20)$$

where k is the ratio of the counting times – usually, but not necessarily, an integer or a reciprocal integer. Obviously R_o is not now necessarily an integer. Equation (4) becomes

$$p(R_o) = \exp\{-(B + T)\} \times \sum_{B_o=0}^{\infty} B^{B_o}T^{R_o+kB_o}/B_o!(R_o + kB_o)!. \quad (21)$$

The sum on the right-hand side of (21) is no longer a hyperbolic Bessel function, but a generalization of it, apparently first studied by Wright (1933, 1935). In Wright's notation

$$\varphi(\rho,\beta:z) = \sum_{l=0}^{\infty} z^l/\Gamma(l + 1)\,\Gamma(\rho l + \beta), \quad (22a)$$

but in more recent publications (for example, Olkha & Rathie, 1971) the relationship with Bessel functions is emphasized by notations like

$$I_\nu^\mu(x) = \sum_{r=0}^{\infty} (x/2)^{\nu+2r}/r!\Gamma(1 + \nu + \mu r). \quad (22b)$$

This reduces to the ordinary I_n for $\mu = 1$, $\nu = n$. In this notation (21) becomes

$$p(R_o) = \exp\{-(B + T)\}(T^{2-k}/B)^{R_o/2}I^k_{|R_o|}\{2(BT^k)^{1/2}\}, \quad (23)$$

reducing to (5) for $k = 1$. Wright's function does not appear to have been tabulated. It is a special case of a much more general class of functions, for which there is an extensive literature (see, for example, Braaksma, 1963), but nothing has been found in a wide but not exhaustive search that is of greater practical help than Wright's (1933) paper. This paper gives an expansion that is asymptotic in B and T, but not in R_o. It is thus analogous to (13) rather than to (9), but it covers the region of interest for the French & Wilson (1978) procedure. In the present notation

$$p(R_o) \simeq \{2\pi(k + 1)(kBT^k)^{1/(k+1)}\}^{-1/2}(T/kB)^{R_o/(k+1)} \times \exp\{[(k + 1)/k](kBT^k)^{1/(k+1)} - S\}, \quad (24)$$

which reduces to (13), as it should, for $k = 1$. On making the substitutions $T = qkB$, $R = (q - 1)kB$, in a fashion analogous to (15), (24) becomes

$$p(R_o) \simeq \{2\pi k(k + 1)q^{k/(k+1)}\}^{-1/2}\,q^{R_o/(k+1)} \times \exp\{[(k + 1)q^{k/(k+1)} - qk - 1]B\}, \quad (25)$$

and the equivalent normal expression is

$$p(R_o) = \{2\pi(q + k)kB\}^{-1/2} \times \exp\{-(R_o/B - qk + k)^2B/2k(q + k)\}. \quad (26)$$

The ratio of expression (25) to the normal expression (26) for $R_o = 0$ is

$$\frac{p(0)\ (\text{Wright})}{p(0)\ (\text{normal})} = \left(\frac{k + q}{k + 1}\right)^{1/2} q^{-k/2(k+1)} \times \exp\left\{\left[-1 - kq + (k + 1)q^{k/(k+1)} + \frac{k(q - 1)^2}{2(k + q)}\right]B\right\}, \quad (27)$$

where the terms have been arranged to make comparison with (17) easy.

As already mentioned, (24) is valid only for small R_o; the second term of Wright's series, omitted in (24), suggests that the condition is $R_o^2 \ll (kBT^k)^{1/(k+1)}$. An expression valid for large R_o can be obtained by the following argument. From formula 6.1.47 of Abramowitz & Stegun (1964)

$$z^{b-a}\Gamma(z + a)/\Gamma(z + b) \simeq 1 + (a - b)(a + b - 1)/2z + \ldots, \quad (28)$$

with a few restrictions on negative values of z. Applying this formula to (21) ($z = R_o$, $a = 1$, $b = kB_o + 1$) gives

$$p(R_o) \simeq [\exp(-S)T^{R_o}/\Gamma(R_o + 1)]\sum_{B_o}[(BT^k/R_o^k)^{B_o}/B_o!] \times \{1 - kB_o(kB_o + 1)/2R_o + \ldots\}. \quad (29)$$

The term in curly brackets can be expressed as

$$\{1 - k(k+1)B_o/2R_o - k^2B_o(B_o - 1)/2R_o + \ldots\},$$

so that with a little manipulation (29) becomes

$$p(R_o) \simeq [T^{R_o}/\Gamma(R_o + 1)] \exp(BT^k/R_o^k - S) \times \{1 - k(k+1)(BT^k/R_o^k)/2R_o - k^2(BT^k/R_o^k)^2/2R_o + \ldots\}. \quad (30)$$

Equation (30) is a rather better approximation than (10) for large R_o, even for $k - 1$; they become identical if $\Gamma(R_o + 1)$ is approximated by Stirling's formula and the terms in BT^k/R_o^k are neglected. The normal approximation (26) approaches zero with increasing R_o more quickly than (30) does.

For various reasons, in particular the conditions for the validity of (28), (30) cannot be applied for R_o negative. If R_o is negative, (21) starts with a lot of zero terms, since $R_o + kB_o$ (being equal to T_o) is integral even if R_o is not, and the factorial of a negative integer is infinite. It is therefore more convenient to take T_o, which may be written in this case

$$T_o = -|R_o| + kB_o, \quad (31)$$

as the index of summation, giving ultimately

$$p(-|R_o|) \simeq [B^{|R_o|/k}/\Gamma(|R_o|/k + 1)] \times \exp[(kBT^k/|R_o|)^{1/k} - S]\{1 + \ldots\}, \quad (32)$$

where the first few terms in the curly brackets could be readily supplied if necessary. Like (30), (32) does not approach zero as rapidly as the normal approximation as $|R_o|$ increases.

4. Fixed-count timing

The probability of a time t being required to accumulate m counts when the true counting rate is λ is given by the so-called gamma distribution

$$p(t)dt = [\lambda(\lambda t)^{m-1} \exp(-\lambda t)/(m-1)!]dt. \quad (33)$$

The normalization is easily checked, since

$$\int_0^\infty x^m \exp(-x)dx = m!. \quad (34)$$

It would naively be supposed that the average value of m/t would be a good estimate of the counting rate λ, but it is in fact slightly biased, and the unbiased estimate of the counting rate is $(m-1)/t$, as is easily verified:

$$\langle (m-1)/t \rangle = (m-1) \int_0^\infty t^{-1} p(t)dt = (m-1)\lambda(m-2)!/(m-1)! = \lambda. \quad (35)$$

The variance of this estimate of the counting rate is similarly found to be

$$\sigma^2\{(m-1)/t\} = \lambda^2/(m-2). \quad (36)$$

The differences introduced by the corrections -1 or -2 are generally negligible, but would not be for counts as low as those proposed by Killean (1967).

In order to make comparison with fixed-time counting as easy as possible, a parallel notation will be used: T is the true counting rate when the diffractometer is set on a reflexion; B is the true counting rate when the diffractometer is set to recieve background; R is the difference $T - B$; T_o is the unbiased estimate of the counting rate when the diffractometer is set to receive a reflexion; B_o is the similar estimate of the background counting rate; R_o is the difference $T_o - B_o$; m_1 is the fixed number of counts used in estimating T_o; t_1 is the experimentally determined time for accumulating m_1 counts; m_2 and t_2 are the analogous quantities for the background. These definitions imply that

$$T_o = (m_1 - 1)/t_1, \quad (37)$$

$$B_o = (m_2 - 1)/t_2, \quad (38)$$

$$R_o = (m_1 - 1)/t_1 - (m_2 - 1)/t_2, \quad (39)$$

$$\sigma^2(R_o) = T^2/(m_1 - 2) + B^2/(m_2 - 2). \quad (40)$$

The probability distribution (36) becomes

$$p(t_1)dt_1 = [T(Tt_1)^{m_1-1} \exp(-Tt_1)/(m_1 - 1)!]dt_1 \quad (41)$$

for the counting time when the diffractometer is set on a reflexion, and

$$p(t_2)dt_2 = [B(Bt_2)^{m_2-1} \exp(-Bt_2)/(m_2 - 1)!]dt_2 \quad (42)$$

when it is set to collect background. It must be remembered that in this section T, B, R, *etc.* are counting *rates*, and not *numbers* of counts, as in §3.

It is not, in fact, difficult to write down the probability distributions of the counting rates T_o and B_o. For T_o, for example,

$$p(T_o)dT_o = p(t_1)\left|\frac{dt_1}{dT_o}\right|dT_o, \quad (43)$$

where $p(t_1)$ is given by (41) and t_1 is to be replaced by its equivalent in terms of T_o from (37). The result is

$$p(T_o)dT_o = \frac{[T(m_1 - 1)/T_o]^{m_1+1}}{(m_1 - 1)!} \times \exp\left\{-\frac{(m_1 - 1)T}{T_o}\right\} \frac{dT_o}{(m_1 - 1)T}. \quad (44)$$

There does not seem to be a generally recognized special name for the distribution (44).

The probability distribution of R_o is obtained by multiplying the distributions (41) and (42) together and integrating over those values of t_1 and t_2 that lead to values of R_o lying between R_o and $R_o + dR_o$. For R_o non-negative, from (39),

$$t_1 = \frac{m_1 - 1}{R_o + (m_2 - 1)/t_2}, \tag{45}$$

$$dt_1 = -\frac{(m_1 - 1)dR_o}{[R_o + (m_2 - 1)/t_2]^2}, \tag{46}$$

so that

$$p(R_o)dR_o = \frac{(m_1 - 1)^{m_1}}{(m_1 - 1)!(m_2 - 1)!} \times \int_0^\infty \left[\frac{T}{R_o + (m_2 - 1)/t_2}\right]^{m_1 + 1} \times (Bt_2)^{m_2 - 1} \times \exp\left\{-\frac{(m_1 - 1)T}{R_o + (m_2 - 1)/t_2} - Bt_2\right\} \times d(Bt_2)d(R_o/T). \tag{47}$$

The integral in (47) is not very tractable, perhaps because the distribution function for T_o (44) and the corresponding distribution for B_o do not possess moments of all orders; only the first $m_1 - 1$ and $m_2 - 1$ exist. The right-hand side of (47) can be expanded in powers of R_o. With q defined by the analogue of the definition used in (25),

$$q = (m_1 - 1)T/(m_2 - 1)B, \tag{48}$$

the series is

$$p(R_o)dR_o = \frac{q^{m_1+1}(m_1 + m_2)!}{(m_1 - 1)!(m_2 - 1)!(1 + q)^{m_1+m_2+1}} \times \frac{dR_o}{(m_1 - 1)T}\left\{1 + (m_1 + m_2 + 1) \times \frac{q}{(1 + q)^2}[(m_2 + 1)q - (m_1 + 1)] \times \frac{R_o}{(m_1 - 1)T} + [(m_1 + m_2 + 2)(m_1 + m_2 + 1)/2!] \times \frac{q^2}{(1 + q)^4}[(m_2 + 2)(m_2 + 1)q^2 - 2(m_1 + 2)(m_2 + 2)q + (m_1 + 1)(m_1 + 2)] \times \frac{R_o^2}{(m_1 - 1)^2T^2} + \ldots\right\}. \tag{49}$$

Unfortunately the series is usable only in a very small range about $R_o = 0$.

The most interesting question is whether the true probability of small positive or small measured-as-negative intensities is greater or less than that given by a normal distribution having the same mean and variance. In general both the true and the normal values of $p(0)$ are messy, but they simplify considerably for $m_1 = m_2, = m$, say. Using Stirling's approximation for the factorials one obtains, with q now T/B,

$$\frac{p(0)\ (\text{true})}{p(0)\ (\text{normal})} = \frac{m}{m - 1}\left(\frac{m}{m - 2}\right)^{1/2} \frac{[2(1 + q^2)]^{1/2}}{q + 1} \times \exp\left[-\frac{(q - 1)^2}{q^2 + 1}\right] \times \exp\left(-m\left\{-\frac{(q - 1)^2}{2(q^2 + 1)} + 2\log_e[\tfrac{1}{2}(q + 1)] - \log_e q\right\}\right), \tag{50}$$

where the terms in q have been arranged so that they reduce to unity for $q = 1$. The initial term in m differs from unity to a negligible extent, except perhaps in Killean's (1967) application. The behaviour of the ratio thus depends on the value of the coefficient of m in the exponential. This has the value zero for $q = 1$, and seems to be negative for all values of q greater than unity, approaching $\frac{1}{2} - \log_e(q/4)$ for q large. The true probability is thus less than the probability given by the normal approximation. For very large values of $|R_o|$ the probability given by the exact expression (47) becomes greater than that given by the normal approximation, but in this region both probabilities are too small to be of practical interest.

5. The central limit theorem

The above discussions have shown that the probability of small positive and small measured-as-negative intensities differs from that to be expected from the normal approximation to the distribution functions. One may therefore have an uneasy feeling that there must be errors in the calculations, for does not the central limit theorem prove that for sufficiently large values of some explicit or implicit parameter n (in the present context the number of counts) all distributions tend to normality? This impression is certainly given by many textbooks, but the situation is far from simple. In the strict sense of the term, the central limit theorem applies to the distribution of the sum of n random variables, and is clearly irrelevant to the present problem: the distribution of the difference of precisely two random variables, each having a known, non-normal, distribution. However, there is a looser sense: the approach to normality of a distribution that can be represented by a Gram-Charlier A (Cramér, 1945, pp. 221–227) or an Edgeworth (Cramér, 1945, pp.

227–231) series. In the Edgeworth form the representation is

$$f(x) = \varphi(x)\{H_0 + \gamma_1 H_3(x)/3! + \gamma_2 H_4(x)/4! + 10\gamma_1^2 H_6(x)/6! + \ldots\}, \quad (51)$$

where x is the standardized variable (actual variable minus the mean, divided by the standard deviation), γ_1 and γ_2 are the coefficients of skewness and excess (kurtosis) (Cramér, 1945, p. 184), $\varphi(x)$ is the normal distribution, and H_k is the Hermite polynomial of degree k (Cramér, 1945, p. 133; He_k in the notation of Abramowitz & Stegun, 1964); H_0 is in fact unity. Asymptotic normality follows from the observation that γ_1 is of the order of $n^{-1/2}$ and γ_2 of the order of n^{-1} (Cramér, 1945, pp. 228–229), and further terms of the series decrease as higher inverse powers of n. Thus, *for fixed* x, functions that can be represented in the form (51) approach the normal distribution $\varphi(x)$ as n is increased. The present problem is, however, rather different, and is in fact twofold:

(i) is (51) a valid representation of the distribution sought, and, if so,

(ii) *for fixed* n, how does $f(x)$ behave as $|x|$ increases?

The second question is readily answered: H_k has x^k as its leading term, so that for fixed n the 'correction' terms in (51) increase without limit as $|x|$ increases, and ultimately dominate the expression for $f(x)$. Unless $f(x)$ happens to be normal to begin with, the representation (50) is far from normal for $|x|$ large (more than a few times the cube root of γ_1^{-1} or the fourth root of γ_2^{-1}).

The first question is more difficult, and turns on the meaning of 'valid'. Cramér (1945, p. 222) postulates the existence of moments of all orders, a condition fulfilled for fixed-time counting but not for fixed-count timing. It seems risky, therefore, to base any arguments on (51) for fixed-count timing. Secondly, for (51) to converge to $f(x)$ the integral

$$\int_{-\infty}^{+\infty} \exp(\tfrac{1}{4}x^2) f(x) \mathrm{d}x \quad (52)$$

must exist (Cramér, 1945, p. 223). This integral is infinite if the asymptotic form (30) is correct for fixed-time counting, so that even in the more favourable case (51) does not converge. The first few terms will thus be a good approximation to the true distribution for $|x|$ small, but the approximation will deteriorate rapidly as $|x|$ increases. All in all, therefore, appreciable deviations from normality in intensity distributions need not be an occasion for surprise.

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