17.X-04 BAYESIAN STATISTICS. By Simon French* and Stuart Oatley, Laboratory of Molecular Biophysics, Oxford University, England.

In interpreting crystallographic results there are generally two sources of information: the experiment itself and data from previous investigations. Conventional statistics does not provide a simple, conceptually clear means of combining these. Bayesian statistics does, however, provide such a framework. To illustrate this we consider procedures for estimating a diffraction peak's intensity from its measured profile. Various methods have been proposed for doing this. However, all ignore some of the available information, thereby reducing the accuracy of the estimation. Moreover, some make assumptions about structure present in the sequence of counts and so produce a large positive bias in the estimates of weak reflections. We present a profile fitting approach based upon the Bayesian three-stage regression model, which we believe overcomes these failings. We discuss the underlying theory, describe briefly its implementation for off-line data reduction, and report on its application to various protein data sets.

* Present address, Department of Decision Theory, University of Manchester, England.

17.X-05 INTENSITY DISTRIBUTIONS IN SPACE GROUPS OF HIGHER SYMMETRY. By Uri Shmueli, Department of Chemistry, Tel-Aviv University, 69978 Ramat Aviv, Israel.

The role of space group symmetry in effects of heterogenous atomic composition of the crystal on the distribution of diffracted intensities has been investigated by statistical methods.

A generalization of the variance of intensity to almost all space groups (Wilson, A.J.C., Acta Cryst. (1978) A34, 986) and an introduction of symmetry- and composition-dependent cumulative distributions (Shmueli, U., Acta Cryst. (1979) A35, 282) indicated a way of attacking the problem and led to a reformulation of intensity statistics and to its extension to all crystallographic symmetries (Shmueli, U. & Wilson, A.J.C., Acta Cryst. (1981); Shmueli, U. & Kaldor, U., Acta Cryst. (1981)), for the case of atoms in general positions and without dispersion.

The probability density functions for the normalized structure amplitude, equivalent to their previously published versions, are given by

$$P_c(|E|)=\left(\frac{2}{\pi}\right)^{\frac{1}{2}}\exp\left(-\frac{|E|^2}{2}\right)\left[1+\sum_{k=2}^{4}\frac{A_{2k}}{2^k(2k)!}H_{2k}\left(\frac{|E|}{\sqrt{2}}\right)+\ldots\right] \quad (1)$$

and

$$P_a(|E|)=2|E|\exp(-|E|^2)\left[1+\sum_{k=2}^{4}\frac{B_{2k}}{(-1)^k k!}L_k(|E|^2)+\ldots\right] \quad (2)$$

for centrosymmetric and non-centrosymmetric space groups respectively; H_{2k} are Hermite and L_k are Laguerre polynomials. The coefficients A_{2k} and B_{2k} are linear in the even moments of $|E|$ which, in their turn, are expressed in terms of functions of atomic scattering factors and even moments of $|J|$, where

$$J(\underset{\sim}{h}) = \sum_s \exp[2\pi i \underset{\sim}{h}^T(P_s\underset{\sim}{r} + \underset{\sim}{t}_s)] \quad (3)$$

is the trigonometric structure factor.

This formulation of the moments $\langle|E|^{2n}\rangle$ is more suitable for a treatment of high symmetries than that employing mixed moments of the real and imaginary parts of J (e.g., Foster, F. & Hargreaves, A., Acta Cryst. (1963) 16, 1124), and leads to concise expressions for A_{2k} and B_{2k} in (1) and (2) respectively.

Numerical values of $\langle|J|^2\rangle$, $\langle|J|^4\rangle$ and $\langle|J|^6\rangle$, required for the evaluation of $\langle|E|^4\rangle$ and $\langle|E|^6\rangle$, are available for all the space groups and $\langle|J|^8\rangle$ can also be computed with the aid of existing algorithms.

Omission of the terms in $\langle|J|^8\rangle$ from A_8 and B_8 reduces the p.d.f.'s (1) and (2) to three-term Edgeworth expansions, approximately asymptotic in the number of atoms in the asymmetric unit. Such expansions may often be sufficiently accurate for a meaningful representation of the effects of symmetry and composition on intensity distributions.

The main results of this work will be summarized and illustrated, and some applications of this statistics to practical problems will be presented.

The author's collaboration with Professors A.J.C. Wilson and U. Kaldor is gratefully acknowledged.

17.X-06 STATISTICS OF RECORDED COUNTS. By J.L. de Boer, Laboratory for Chemical Physics, Rijksuniversiteit Groningen, Nijenborgh 16, 9747 AG Groningen, The Netherlands.

Probability distributions for a measured reflection intensity $R_o=T_o-B_o$, where T_o and B_o are the peak and background intensity respectively and R, T and B the "true" number of counts, have been studied by different authors (see, for instance, A.J.C. Wilson (1978) Acta Cryst. A34, 474). Since R_o, negative values included, is an unbiased estimator of R, it has been proposed (Hirschfeld & Rabinovich (1973), Acta Cryst. A29, 510) to base structure determinations on R_o rather than on the R_o^2 values, which for weak reflections are not unbiased estimators of the true structure factors (Ibers & Hamilton (1964), Acta Cryst., 17, 781). However, the calculation of deformation maps for accurate electron density studies requires the use of R_o^2. A practical way to reduce the probability of R_o being negative is to make the background as small as possible. Probability distributions for different backgrounds will be shown and will be compared with sets of measurements in which the background is reduced by use of monochromator.

Another source of error in the deformation density maps are the very strong reflections. Unless large counting times are spent on these reflections, their R_o^2 values, which in this case may be considered as unbiased estimates, have large standard deviations. Practical limitations may prevent to make $\sigma(R_o^2)$ independent of R. Recent experimental results in which unexpected apparatus instabilities played a role, will be shown.