

given value of ρ in the given equation gives $\varphi(y) = 1$, not $\varphi(y) = 1/\sigma_i^2$, though the latter result would be correct. Nowhere is y defined, so the reader has to rely on implication in the presence of an error. Moreover, the same symbol is also used for observations before the formation of observational differences.

Having convinced oneself that y corresponds to R/σ (and that a minor error is present) one finds examples of ρ and φ on page 81 which are related according to $\varphi = (1/y)(\partial\rho/\partial y)$ suggesting that y corresponds to R after all. Whether y is R or R/σ , of course, is immaterial if σ_i is independent of i , but we expect a general treatment here.

Despite these criticisms of presentation this chapter contains much that is good and is full of ideas and suggestions which may be extremely helpful when carefully applied. This is particularly true in relation to techniques of solution and to the recognition and handling of local minima.

Chapter 7 is concerned with the statistics of the estimation of errors and provides a comprehensive treatment of the normal error case together with some useful comments relating to non-normal distributions and robust/resistant treatments of these. My only criticisms here are minor ones in that the procedure recommended on page 96 for estimating σ should be avoided when σ/μ is very small since the procedure, which is analogous to determining the smallest side of a right-angled triangle by measuring the two longer sides, becomes very susceptible to round-off errors in computation when σ/μ is small. The other is in the presentation of the χ^2 distribution on page 100, where some explanation of χ as a radius in a ν -dimensional hyperspace containing a spherical Gaussian distribution would be conceptually helpful. Appendix D, however, which deals with the associated algebra, is excellent.

Chapter 8, on significance and accuracy, gives a very good account of correlation amongst the parameters of a problem, together with some useful hints on how to avoid or minimise the effects of correlation by a suitable choice of parameters in the first place. However, it stops short of treatments which depend on determining eigenvalues and eigenvectors of the Hessian – an approach which, though more expensive, may be relied on to characterise fully the inter-dependencies of the parameters and to produce uncorrelated shifts of the transformed variables. This is alluded to in the example of the use of Chebychev polynomials, but not developed for the general case. The discussion of the possible effects of unmodelled parameters is most enlightening.

The final chapter, on constrained crystal-structure refinement, discusses this topic mainly in terms of the proper parameterisation of the problem and draws on the work of previous chapters to explain tests, including Hamilton's R -factor ratio test, which may be applied to determine the necessity or otherwise of including certain parameters in a model. Quite properly in my view, discussion of Lagrange undetermined multipliers is avoided in preference to the use of constraint matrices which serve to describe the problem in terms of a subspace section of parameter space, though I would like to have seen this topic expanded a little further. I also felt that it would have been appropriate here to relate penalty functions (touched on in chapter 6) to the formal representation of an *a priori* probability density distribution in parameter space and to show that their use leads formally to an *a posteriori* probability density

distribution with variances and covariances properly described by the matrix which is the sum of the usual Hessian and the matrix of coefficients in the penalty functions.

Refinement of the orientation of rigid bodies in terms of Eulerian angles is discussed here and some of the work of chapter 1 is repeated, but with sign reversals in each of the angles (which presumably arise from the distinction between rotating an object and rotating the axes to which the object is referred, but the sign change appears without comment).

Much of the emphasis throughout the book is on statistical aspects and it is in this connection that I think the book is particularly good. This is supported by a number of appendices which develop the basic theory and also provide Fortran source code for a number of useful statistical functions.

Although I was conscious of a number of misprints, I consider it very good value at DM 55.

ROBERT DIAMOND

MRC Laboratory of Molecular Biology
Hills Road
Cambridge CB2 2QH
England

Acta Cryst. (1984). A40, 87

Crystallographic statistics: progress and problems.

Edited by S. RAMESESHAN, M. F. RICHARDSON and A. J. C. WILSON. Pp. 313. Bangalore: Indian Academy of Sciences, 1982. Price US\$ 18 (£9) for institutions; US\$ 9 (£5) for individuals.

This volume contains the proceedings of the symposium on Progress and Problems in Crystallographic Statistics held prior to the Twelfth Congress of the International Union of Crystallography, Ottawa, 1981. In a short introduction A. J. C. Wilson draws a brief historical background of the beginning of crystallographic statistics. A good overview of the statistical properties of the intensities of X-rays scattered by a crystal is given by H. Hauptman. The main topics: Bayesian statistics, intensity statistics, measurability of Bijvoet differences, statistics of recorded counts, variations on least-squares and Wiener-Kolmogorov methods are treated in twelve subsequent full papers and three abstracts; they give the present state of knowledge, as well as provide a useful reference source for the specialist. In addition, the extended subject index makes the book very useful. The book is of interest for scientists who carry out structure-determination work in all fields of crystallography. However, the more elaborate treatment of the intensity statistics requires a high mathematical level; the non-specialist will find a general introduction in the excellent book by Srinivasan & Parthasarathy: *Some statistical applications in X-ray crystallography*, Pergamon Press, Oxford, 1976.

The low price of the book, the remarkable printing and the solid binding with hard plastic cover make it an excellent purchase.

PETER ENGEL

Laboratory of Crystallography
University of Bern
Switzerland