way to consider crystallographic refinement although to the present day it has not been used in practical applications to its full power. Stage One is associated with the observational error, typically quantum counting statistics for diffractometer measurements. Stage Two is concerned with physical modelling and its error - not only the relation between atomic parameters and calculated intensities but also the error associated with this modelling. Stage Three embodies prior knowledge of parameters - their possible values and dispersion. Stage One is very familiar and is the only error source appearing in a Frequentist analysis. Choice and adjustment of weighting schemes are closely related to stage Two. Use of restaints is clearly associated with stage Three.

Due to improvements in equipment and experimental technique, the extraction of physical and chemical information (and their error estimates) from many diffraction experiments, either single crystal or powder, is currently limited by model deficiences - systematic errors. Two courses of action are possible: Improve the models or explicitly quantify the poorness of the existing ones. The latter course must be undertaken using the Bayesian Philosophy.

17.X-12 REPORT ON THE WORK OF THE SUBCOMMITTEE ON STATISTICAL DESCRIPTORS. By D. Schwarzenbach, Institut de Cristallographie, Université de Lausanne, Bâtiment des Sciences Physiques, CH - 1015 Lausanne, Switzerland

The Subcommittee on Statistical Descriptors was established by the IUCr Commission on Crystallographic Nomenclature. The members are D. Schwarzenbach (chairman), H.D. Flack, W. Gonschorek, R.E. Marsh, E. Prince, B.E. Robertson and J.S. Rollett. Ex-officio members S.C. Abrahams and A.J.C. Wilson contributed actively to the work. The terms of reference are *to examine the validity of current statistical approaches used in estimating the variances in crystallographic quantities and to make recommendations for an improved methodology that rests securely on sound modern statistical theory and that can be widely adopted by the crystallographic community.* This ambitious programme may be surprising to some since there exists a vast literature on probability and statistics, and many of our undergraduate students are required to take courses in these disciplines. However, concern about the relevance of statistical theory as taught nowadays is widespread among experimentalists, be they crystallographers or particle physicists. Their problems are not confined to procedural issues, but have an important philosophical component originating from the need to justify the unavoidable lack of rigour with respect to mathematical theory in the treatment of experimental data. For this reason, one of the important discussions of the Subcommittee concerns the two alternate interpretations of probability, the *frequentist* and the *Bayesian* one. Another issue is the definition and use of the terms *model* and *observation*. Everybody agrees that the model, i.e. the conjecture about the physical reality used to interprete the data, comprises not only the crystal structure, but also data reduction procedures. The statement that *corrected observations and in particular structure amplitudes are not observed quantities* is of fundamental importance to some, and of minor consequence to others. In any case, recommendations of immediate value to practicing crystallographers cannot dispense with data treatment. Procedures to obtain mean values of symmetry-equivalent data and corresponding realistic variances become then important. Hotly debated were the kind of corrected observations which should be refined upon, in particular $|F|$ or $|F|^2$. The discussion of realistic weighting schemes to be used in least squares, and related issues such as the treatment of negative net intensities and the effects of neglecting weak reflections, makes it clear that variances of observations and corresponding weights are necessarily estimated from the observations themselves. Any weighting scheme based on the observed quantities results in bias of the refined parameters which might be reduced by weights computed by a combination of observed and calculated quantities. A preliminary report contains (a) a directory of statistical terms established for use by experimentalists; (b) a description of the statistical basis of refinement procedures and the Bayesian interpretation of statistics; (c) a section on the choice and significance of weighting schemes and (d) recommendations, some of which are easily implemented.

17.1-1 SIMULTANEOUS SEARCH FOR SYMMETRY-RELATED MOLECULES IN PATTERSON SPACE. By Christer E. Nordman, Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109, USA.

In Patterson-space rotational search, the intramolecular vector set, or self-Patterson, of a known molecule or fragment is rotated to find the best fit to the Patterson, P. In translational search, an intermolecular vector set, or cross-Patterson, is correspondingly translated. New procedures, mainly for macromolecules, have been developed in which the search vector set is represented by a continuous vector density distribution of the search model. For rotation search, the self-Patterson is computed as the Patterson of a (triclinic) structure consisting of the known model placed in an orthogonal cell large enough to yield the self-Patterson free from intermolecular overlap. The vector density is transferred to a search grid of points lying on concentric spherical surfaces. This search grid is placed at the origin of P, and rotated through the three Euler angles to search for optimal fit. In non-triclinic crystals two (monoclinic), four (orthorhombic), or more self-Pattersons are embedded in P; these are related to each other by crystallographic symmetry axes. The method permits simultaneous search for all these self-Pattersons. At each search step the symmetry-related self-Patterson(s) are retrieved by two-dimensional interpolation on the spherical surfaces of the search grid. The sum of these two, four, or more copies of the self-Patterson is then compared to P. For translation search, the oriented model is placed in an extended crystal cell such that the computed Patterson yields separated self- and cross-Patterson regions, evaluated on a grid which matches that of P. The self-Patterson is subtracted from P, and the search done by comparing appropriate sums of overlapping model cross-Pattersons to P. Tests with myoglobin and two forms of superoxide dismutase will be described.