

The conjugate axes are chosen by taking each vector \mathbf{l} parallel to a path vector \mathbf{s} for the step. In the first step the rotation is about the axis of steepest descent, defined by the couple \mathbf{g} :

$$\mathbf{s}_1 = \mathbf{g}_1. \quad (13)$$

Later paths each depend on the previous path and couple according to the relation

$$\mathbf{s}_{p+1} = \mathbf{g}_{p+1} + (\mathbf{g}_{p+1}^2 / \mathbf{g}_p^2) \mathbf{s}_p. \quad (14)$$

After each group of three successive paths the axis is once again chosen parallel to the path of steepest descent. The process terminates when the couple vanishes or the last angle of rotation falls below a set value.

In practice E is not a simple quadratic function. Furthermore, although infinitesimal rotations commute and form a vector space, finite rotations do not. There are however two good reasons for expecting that conjugate gradients should yield a rapidly converging solution in spite of these difficulties. The first is that every finite rotation applied, according to (11), leads to the exact minimum of E about that axis in just one step. The second is that when the orientation is close to the correct solution E does become a well-behaved quadratic function of the small rotation angles, and the concept of conjugate axes becomes a very good approximation.

Tests with typical sets of atomic coordinates show that five to eight iterations are usually sufficient to reduce the last rotation below 10^{-10} rad. Given the original \mathbf{U} matrix, the calculation of \mathbf{R} takes only 0.0032 s and 32 K bytes of store on an IBM 370/165. This is about one-third of the time taken by the previous method (McLachlan, 1979). A version of Kabsch's method, programmed by Dr Arthur Lesk, took 0.0050 s for the same task.

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Non-zero values of odd mixed moments in intensity statistics. By F. FOSTER, *Department of Mathematics, University of Manchester Institute of Science and Technology, Manchester M60 1QD, England*, A. HARGREAVES, *Department of Pure and Applied Physics, University of Manchester Institute of Science and Technology, Manchester M60 1QD, England*, U. SHMUELI, *Department of Chemistry, University of Tel Aviv, Ramat Aviv, 69978 Tel Aviv, Israel*, and A. J. C. WILSON, *Department of Physics, University of Birmingham, Birmingham B15 2TT, England*

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Abstract

Foster & Hargreaves [*Acta Cryst.* (1963), **16**, 1127], in discussing partial mixed moments of structure amplitudes, remark in passing 'For the triclinic, monoclinic and orthorhombic space groups the partial moments m_{pq} are zero when either p or q is odd, but for higher symmetries non-zero moments exist for p odd and q even'; the remark is repeated without comment by Srinivasan & Parthasarathy [*Some Statistical Applications in X-ray Crystallography* (1976).

Oxford: Pergamon Press]. Shmueli & Wilson failed to find any such non-zero moments among the general reflexions for any space group, and the problem has therefore been re-examined. Non-zero odd mixed moments are often found to occur in the *plane* groups with threefold or sixfold rotors, and hence in the *hk0*, but not the *hkl*, reflexions in *space* groups with trigonal or hexagonal symmetry. Details will be given in a forthcoming paper by Shmueli & Kaldor.

All information is given in the *Abstract*.