For our intensity data with $N = 5320$, $M = 9$ we find $d = 1{\cdot}997$, $4 - d = 2{\cdot}003$ and the percentage point 0·1%: $Q = 1{\cdot}918$, 1%: $Q = 1{\cdot}939$, 5%: $Q = 1{\cdot}958$. Thus we cannot reject the null hypothesis of serial independence, *viz.* we find no evidence of serial correlation in our data set.

In conclusion it would seem desirable to incorporate the test for serial correlation into crystallographic least-squares programs as a means of detecting unsuspected errors in the data set. In the main, these could either be associated with the treatment of the reference reflections or be due to any long-term instability in the measuring apparatus or crystal.

APPENDIX

Proof of statement that even where there is serial correlation the ordinary least-squares method gives unbiased estimates of the parameters

Consider the simple linear relationship

$$Y_t = \alpha + \beta X_t + U_t, \qquad \text{(A1)}$$

where α and β are parameters and U_t is a disturbance or error term. It is assumed for simplicity that U_t follows a first-order Markov auto-regressive scheme, *i.e.*

$$U_t = \rho U_{t-1} + e_t$$

where $|\rho| < 1$ and e_t is an individual error disturbance term with the expectations that

$$\begin{aligned} E(e_t) &= 0 \\ E(e_t.e_{t+s}) &= \sigma_e^2 \text{ when } s = 0 \\ &= 0 \quad \text{when } s \neq 0 \end{aligned} \Bigg\} \text{for all } t.$$

Then

$$\begin{aligned} U_t &= \rho(U_{t-1}) + e_t \\ &= \rho(\rho U_{t-2} + e_{t-1}) + e_t \\ &= \rho^2(\rho U_{t-3} + e_{t-2}) + \rho e_{t-1} + e_t \\ &= \rho^3(\rho U_{t-4} + e_{t-3}) + \rho^2 e_{t-2} + \rho e_{t-1} + e_t \\ &= \rho^4(\rho U_{t-5} + e_{t-4}) + \rho^3 e_{t-3} + \rho^2 e_{t-2} + \rho e_{t-1} + e_t \end{aligned}$$

and so on in this iterative manner.

$$U_t = e_t + \rho e_{t-1} + \rho^2 e_{t-2} + \rho^3 e_{t-3} + \ldots + \rho^r e_{t-4} + \ldots$$

or

$$U_t = \sum_{r=0}^{\infty} \rho^r e_{t-r}.$$

Since

$$E(e_t) = 0 \quad \text{(assumed above)},$$

it follows that

$$E(U_t) = E\left[\sum_{r=0}^{\infty} \rho^r e_{t-r}\right] = 0.$$

Taking expectations of (A1), then

$$E(Y_t) = E(\alpha + \beta X_t + U_t),$$
$$E(Y_t) = E(\alpha) + E(\beta X_t) + E(U_t)$$

or

$$E(Y_t) = \alpha + \beta\mu_x + 0,$$

i.e. we still get unbiased estimates of the parameters even when U_t follows an auto-regressive scheme.

References

BECKER, P. J. & COPPENS, P. (1974). *Acta Cryst.* A**30**, 129–153.
BECKER, P. J. & COPPENS, P. (1975). *Acta Cryst.* A**31**, 417–425.
DURBIN, J. & WATSON, G. S. (1950). *Biometrika*, **37**, 409–428.
DURBIN, J. & WATSON, G. S. (1951). *Biometrika*, **38**, 159–178.
THEIL, H. & NAGAR, A. L. (1961). *J. Am. Stat. Assoc.* **56**, 793–806.
XRAY system (1976). Edited by J. M. STEWART. Technical Report TR-446, Computer Science Center, University of Maryland.

Acta Cryst. (1980). A**36**, 496

A new least-squares refinement technique based on the fast Fourier transform algorithm: *erratum*. By

RAMESH C. AGARWAL,* *IBM T. J. Watson Research Center, Yorktown Heights, NY* 10598, *USA*

(*Received* 12 *December* 1979)

Abstract

In Agarwal [*Acta Cryst.* (1978), A**34**, 791–809], equation (61) should read

$$c_3 = 2C_m^1 C_{m'}^2.$$

All information is given in the *Abstract.*

* Present address: Centre for Applied Research in Electronics, Indian Institute of Technology, New Delhi 110029, India.

0567-7394/80/030496-01$01.00