

For our intensity data with  $N = 5320$ ,  $M = 9$  we find  $d = 1.997$ ,  $4 - d = 2.003$  and the percentage point 0.1%:  $Q = 1.918$ , 1%:  $Q = 1.939$ , 5%:  $Q = 1.958$ . 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

$$Y_t = \alpha + \beta X_t + U_t, \quad (A1)$$

where  $\alpha$  and  $\beta$  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

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

Then

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

$= \rho^4(\rho U_{t-5} + e_{t-4}) + \rho^3 e_{t-3} + \rho^2 e_{t-2} + \rho e_{t-1} + e_t$   
and so on in this iterative manner.

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

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.

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

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#### Abstract

In Agarwal [*Acta Cryst.* (1978), **A34**, 791–809], equation (61) should read

$$c_3 = 2C_m^1 C_m^2.$$

All information is given in the *Abstract*.

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