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

\[
Y_t = \alpha + \beta X_t + U_t,
\]

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

\[
E(e_t) = 0
\]

\[
E(e_t, e_{t+s}) = \sigma^2 \quad \text{when } s = 0
\]

\[
= 0 \quad \text{when } s \neq 0
\]

for all \( t \).

Then

\[
U_t = \rho(U_{t-1} + e_t)
\]

\[
= \rho(\rho U_{t-2} + e_{t-1}) + e_t
\]

\[
= \rho^2(\rho U_{t-3} + e_{t-2}) + \rho e_{t-1} + e_t
\]

\[
= \rho^3(\rho U_{t-4} + e_{t-3}) + \rho^2 e_{t-2} + \rho e_{t-1} + e_t
\]

and so on in this iterative manner.

\[
U_t = e_t + \rho e_{t-1} + \rho^2 e_{t-2} + \rho^3 e_{t-3} + ... + \rho^t e_{t-t} + ...
\]

or

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

Since

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

it follows that

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

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**


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

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**Abstract**

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

\[
c_3 = 2C_\alpha^2 C_m^2.
\]

All information is given in the Abstract.

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