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Estimation of Semivariograms by the Maximum Entropy Method[1]

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A wide variety of semivariograms may be represented in terms of a first- or second-order autoregressive (AR) process, and the nugget effect may be included by use of a moving average (MA) process. The weighting parameters for these models have a simple functional dependence on the value of the sill and the semivariance at the first and second lag. These may be estimated either graphically from the semivariogram or directly from the computed values. Improved spectral estimates of geophysical data have been obtained by the use of the "maximum entropy method," and the necessary equations were adapted here for the estimation of the weighting parameters of the AR and the MA processes. Comparison among the semivariograms obtained for the ideal case, the observed case, and the estimated case for artificial series show excellent correspondence between the ideal and estimated while the observed semivariogram may show marked divergence.

KEY WORDS: semivariograms, autoregressive process, maximum entropy method.

INTRODUCTION

Much geological data is collected in the form of traverses whether these be from an adit in a mine, a series of outcrops along a stratigraphic unit, or a well log of a drill hole. As a result, the estimation of the semivariogram for such traverses is of considerable importance. Recently, it has been shown that a wide variety of semivariograms can be represented in terms of three models (Sharp, 1981): a first-order autoregressive (AR) process, ARMA (1 0), a second-order AR process, ARMA (2 0), and a mixed first-order moving average (MA) process with a first-order AR, ARMA (1 1). The use of these models allows for the rapid generation of a wide variety of artificial series which can be used to simulate geological traverses. For this reason, the parameter estimation for these models becomes greatly interesting. For many purposes, a graphical estimate of the parameters will prove satisfactory. However, a more objective estimation procedure would be desirable. The recognition that improved spectral estimates can be ob-

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tained for short data records by the "maximum entropy method" suggests that this procedure might also prove reliable for parameter estimation in the ARMA modeling of semivariograms.

A geologist will usually view the variance structure first as a one-dimensional space series and then try to generalize his understanding into two or three dimensions. Although procedures for the simulation of one-dimensional patterns have been established for some time, significant advances have recently been made in multidimensional time and space series analysis (Ripley, 1981, p. 88). In fact, if the variance structure is understood for a series of traverses in different directions, the results can be converted into an equivalent multidimensional space or time series representation (Taneja and Aroian, 1980; Perry and Aroian, 1979).

ESTIMATION OF SEMIVARIOGRAMS

The semivariance of a traverse (Clark, 1979, p. 92) may be defined as

$$\gamma_h^* = \frac{1}{2} \sum_{i=1}^{N-h} (g_i - g_{i+h})^2/(N-h)$$

where γ_h^* is the observed semivariance for lag h, and $g_1, g_2, g_3, \ldots, g_N$ represent observed sample values such as grade, N is the total number of equally spaced observations, while the autocovariance of the traverse (Dijkstra, 1976) may be defined as

$$s_h^2 = [1/(N-h-1)] \sum_{i=1}^{N-h} (g_i - \bar{g})(g_{i+h} - \bar{g})$$

where s_h^2 is the observed autocovariance for lag h, and $\bar{g}$ is the average grade. If the traverse is sufficiently long and stationary then

$$\gamma_h^* = s_0^2 - s_h^2$$

(Jowett, 1955, p. 161). A plot of s^2 versus h yields a covariogram while a plot of γ^* versus h yields a semivariogram. These variables may also be conveniently expressed in terms of the autocorrelation, ρ, by

$$s_h^2 = s_0^2 \rho_h, \qquad \text{and}$$

$$\gamma_h^* = s_0^2(1 - \rho_h) = C(1 - \rho_h)$$

where C is the sill of the semivariogram.

In time series analysis, a series of linear models has been developed for random processes (Fuller, 1976). Of these models (Box and Jenkins, 1970, p. 51), three are of particular interest

1. a first-order autoregressive process, ARMA (1 0), given by

$$g_i = \phi g_{i-1} + \epsilon_i$$

2. a mixed first-order autoregressive and moving average, ARMA (1 1), given by

$$g_i = \phi g_{i-1} + \epsilon_i - \theta \epsilon_{i-1}$$

3. a second order autoregressive process, ARMA (2 0), given by

$$g_i = \phi_1 g_{i-1} + \phi_2 g_{i-2} + \epsilon_i$$

where ϕ and θ are weighting parameters and ϵ_i is a random impulse. The examination of semivariograms of both artificial and observed series shows that a wide variety can be fitted to one of these three models (Sharp, 1981).

An important characteristic of the ARMA models is the well-defined recursive relations that exist for finding the autocorrelation as a function of the lag, h, and the weighting parameters ϕ and θ (Table 1). As a consequence, the semivariogram may be generated recursively if estimates are made of sill and of the weighting parameters. In turn, the weighting parameters depend solely on estimates of ρ_1 and ρ_2 (Table 2), and these may be determined from the observed variances using

$$\rho_1 = (C - \gamma_1)/C = s_1^2/s_0^2, \qquad \text{and}$$

$$\rho_2 = (C - \gamma_2)/C = s_2^2/s_0^2$$

For most exponential and transitive types only a knowledge of ρ_1 is needed to determine the value of ϕ so that one need only observe the overall variance, C, or s_0^2, and the variance at the first lag, γ_1^* or s_1^2. In those cases where a nugget effect is present or the semivariogram shows pseudo-periodicity the variance at the second lag γ_2^* or s_2^2 will be needed. For initial fitting, the standard estimates

Table 1. Recursive Relations for the Autocorrelation of Some Random Models[a]

ARMA (1 0)	$\rho_h = \phi\rho_{h-1}, h \geqslant 1$
	$\rho_0 = 1$
ARMA (1 1)	$\rho_h = \phi\rho_{h-1}, h \geqslant 2$
	$\rho_1 = (1 - \phi\theta)(\phi - \theta)/(1 + \theta^2 - 2\phi\theta)$
ARMA (2 0)	$\rho_h = \phi_1\rho_{h-1} + \phi_2\rho_{h-2}, h \geqslant 2$
	$\rho_1 = \phi_1/(1 - \phi_2)$
	$\rho_0 = 1$

[a]Box and Jenkins, 1970, p. 69, 57, 77, 59.

Table 2. Calculation of the Weighting Parameters of Some Random Processes from Estimates of the Autocorrelation[a]

1. Exponential and transitive semivariograms without a nugget effect.

   Model = ARMA (1 0).

$$\phi = \rho_1, \quad \text{where} \quad 0 \leqslant \phi \leqslant 1$$

2. Exponential and transitive semivariograms with a nugget effect.

   Model = ARMA (1 1).

$$\phi = \rho_2/\rho_1, \quad \text{and}$$
$$\theta = [-B - (B^2 - 4)^{1/2}]/2, \quad \text{where}$$
$$B = (1 + \phi^2 - 2\phi\rho_1)/(\rho_1 - \phi), \quad \text{and}$$
$$0 \leqslant \phi \leqslant 1$$
$$-1 \leqslant \theta \leqslant 1$$

   For this model to be valid, one must have $\rho_1 < \phi$ and $B < -2$.

3. Continuous (mixed exponentials) or pseudo-periodic semivariograms without nugget effect.

   Model = ARMA (2 0).

$$\phi_1 = \rho_1(1 - \rho_2)/(1 - \rho_1^2)$$
$$\phi_2 = (\rho_2 - \rho_1^2)/(1 - \rho_1^2), \quad \text{where}$$
$$0 \leqslant \phi_1 \leqslant 2 \quad \text{and} \quad -1 \leqslant \phi_2 \leqslant 1$$

[a]Box and Jenkins, 1970, p. 58, 77-78, 59-60.

of the semivariance will be adequate, or in those instances where a real periodicity is present graphically smoothed estimates may be prefered.

When an observed series is to be modeled and the results used to generate an artificial series which will then simulate the original, an estimate must also be made of the variance of the random impulse (residual variance). Here again an important feature of the ARMA models is the ease with which this variance (Table 3) can be estimated once the weighting parameters and the total variance have been estimated.

Table 3. Residual Variance of Some Random Processes[a]

ARMA (1 0)	$s_r^2 = s_0^2/(1 - \phi^2)$
ARMA (1 1)	$s_r^2 = s_0^2(1 - \phi^2)/(1 + \theta^2 - 2\phi\theta)$
ARMA (2 0)	$s_r^2 = s_0^2(1 - \phi_2)/(1 + \phi_2)((1 - \phi_2)^2 - \phi_1^2)$

[a]Box and Jenkins, 1970, p. 58, 193, 62.

ESTIMATION BY THE MAXIMUM ENTROPY METHOD

The maximum entropy method or Burg Scheme was originally developed to improve spectral estimates of geophysical data (Burg, 1967). Intensive testing (Lacoss, 1971, p. 670) has shown it to give more reliable estimates of the variance and better resolution than conventional methods particularly when the data records are of short length. In this procedure the AR parameters are calculated recursively by running an AR model in a backward and forward direction over the data such that the residual variance is a minimum (Ulrych, 1972).

The necessary relationships for the ARMA models were adapted from a detailed description of the algorithm developed for spectral analysis (Andersen, 1974) and converted for use in estimating the semivariograms. The least-squares relationships needed for the ARMA (1 0) and the ARMA (1 1) models (Andersen, 1974, eq. for a_{11}) are

$$\phi = \rho_1 = 2 \sum_{i=1}^{N-1} g_i g_{i+1} \Big/ \sum_{i=1}^{N-1} (g_i^2 + g_{i+1}^2), \qquad \text{and}$$

$$\rho_2 = 2 \sum_{i=1}^{N-2} g_i g_{i+2} \Big/ \sum_{i=1}^{N-2} (g_i^2 + g_{i+2}^2)$$

For the ARMA (2 0) model, the necessary relationships (Andersen, 1974, eqs. 7, 8a, 8b, and 5) are

$$\phi_2 = 2 \sum_{i=1}^{N-2} B_i B_i' \Big/ \sum_{i=1}^{N-2} (B_i^2 + B_i'^2), \qquad \text{where}$$

$$B_i = g_i - \rho_1 g_{i+1}$$

$$B_i' = g_{i+2} - \rho_1 g_{i+1}, \qquad \text{and}$$

$$\phi_1 = \rho_1 - \phi_2 \rho_1$$

ESTIMATION OF ARTIFICIAL SERIES

A number of artificial series were generated by assigning selected values to the weighting parameters of the autoregressive processes. The random impulse, ϵ_i, was computed using a uniform pseudo-random number generator with shuffling (IMSL, 1980, routine GGUW) which was converted to normal deviates by use of the inverse normal function (IMSL, 1980, routine MDNRIS). From the assigned weighting parameters, the ideal semivariance was obtained from the recursion formulas while the observed semivariance was calculated from the generated artificial series, and the results plotted as semivariograms (Fig. 1). From the artificial series estimates of the weighting parameters were made using the "maximum entropy method" and these parameters were then used to obtain

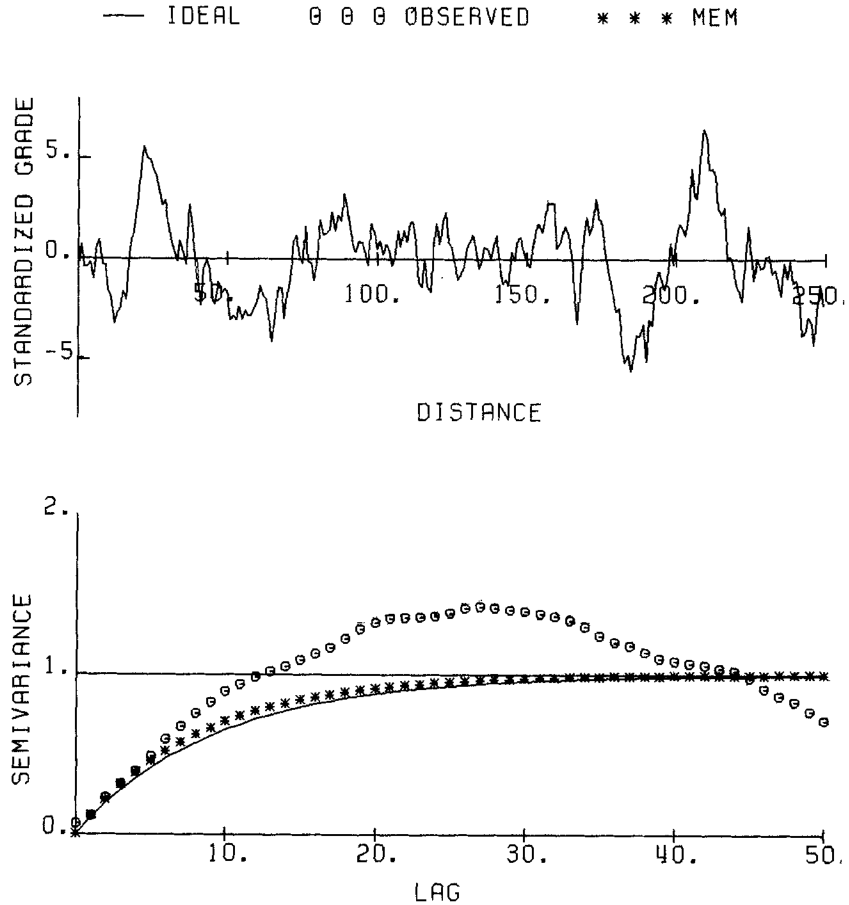

Fig. 1. Ideal, observed, and estimated semivariograms for the ARMA (1 0) process: $g_i = 0.90g_{i-1} + \epsilon_i$. The observed semivariogram was obtained from an artificial series using the pseudo-random number generator GGUW with the seed 4685655. Notice how the observed variogram wanders above both the ideal and the one estimated by the maximum entropy method (MEM $\phi = 0.89$).

an estimated semivariogram by use of the recursion relations. It was plotted and compared with both the ideal and the observed (Fig. 1.)

For a first-order autoregressive process, the curvature of the ideal semivariogram will be exponential (Fig. 1 and 2). Notice the marked deviations that may occur between the observed and the ideal cases because of the limited length of the series. Yet, the estimated semivariogram obtained by calculating the weighting parameters by the maximum entropy method agrees quite well with the ideal semivariogram. Similar nice agreement was found in the case of a

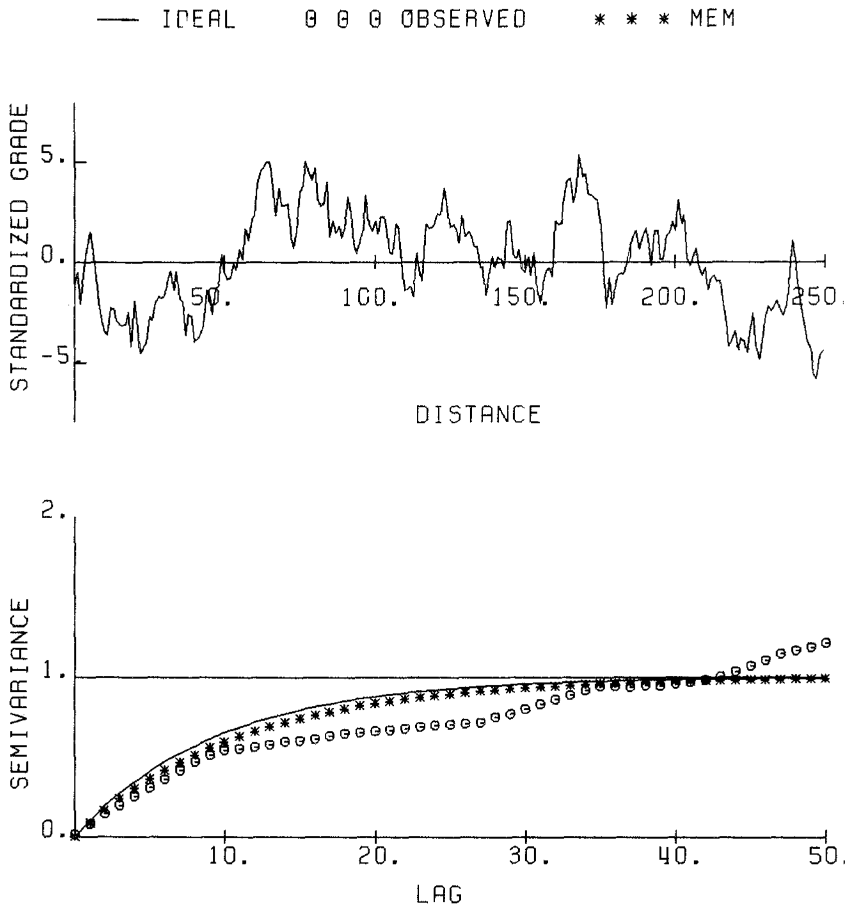

Fig. 2. Ideal, observed, and estimated semivariograms for the ARMA (1 0) process: $g_i = 0.90g_{i-1} + \epsilon_i$. The observed semivariogram was obtained from an artificial series using the generator GGUW and the seed 8224897. Notice how the observed variogram wanders below both the ideal and the estimated (MEM $\phi = 0.91$).

mixed first-order AR and first-order MA (Fig. 3), a second-order AR-mixed exponential (Fig. 4), and a second-order process showing pseudo-periodicity (Fig. 5).

ESTIMATION OF OBSERVED SERIES

With the results of the simulations "in hand," an attempt was made to use these models to estimate some experimental semivariograms. For this purpose,

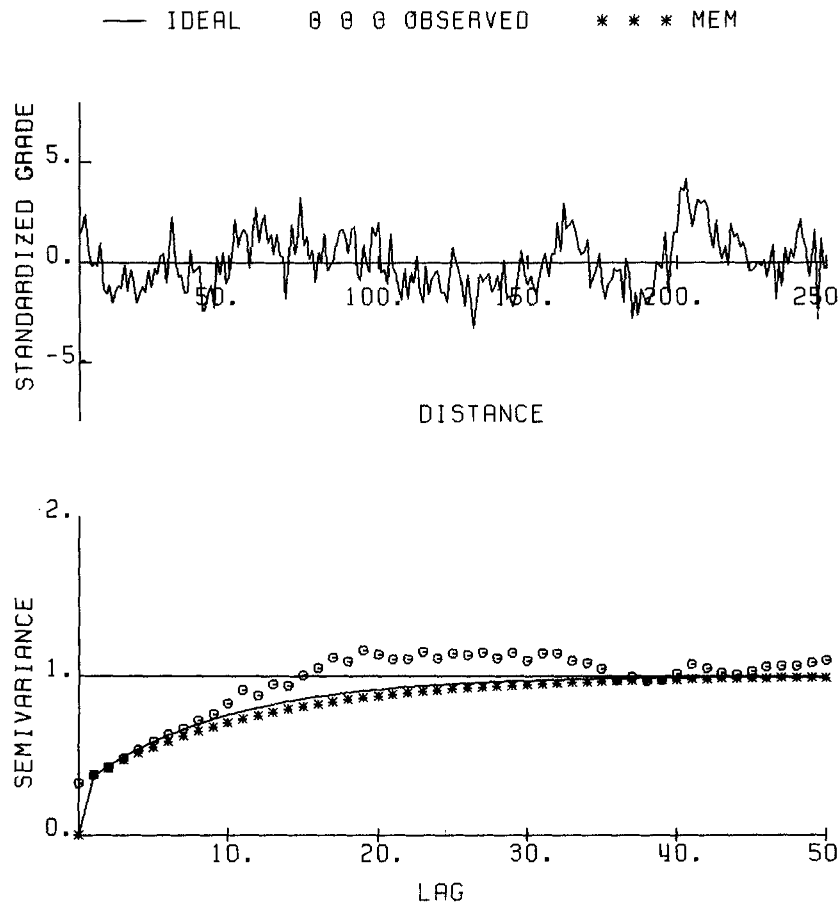

Fig. 3. Ideal, observed, and estimated semivariograms for the ARMA (1 1) process: $g_i = 0.90g_{i-1} + \epsilon_i - 0.50\epsilon_{i-1}$. The observed semivariogram was obtained from an artificial series using the generator GGUW and the seed 7822323. Notice the presence of a distinct nugget effect. The estimated MEM parameters are $\phi = 0.92$ and $\theta = 0.56$.

observed series from a bore hole in the Copper Mountain (Wyoming) uranium district and mine data from the Eagle Copper vein in British Columbia were utilized.

The observations from the bore hole through granite at Copper Mountain (CM-1) consisted of well log analyses for K, U, and Th obtained with a γ ray spectrometer. The observed semivariogram of the K analyses (Fig. 6) shows a general exponential curvature with superimposed undulations. This diagram may

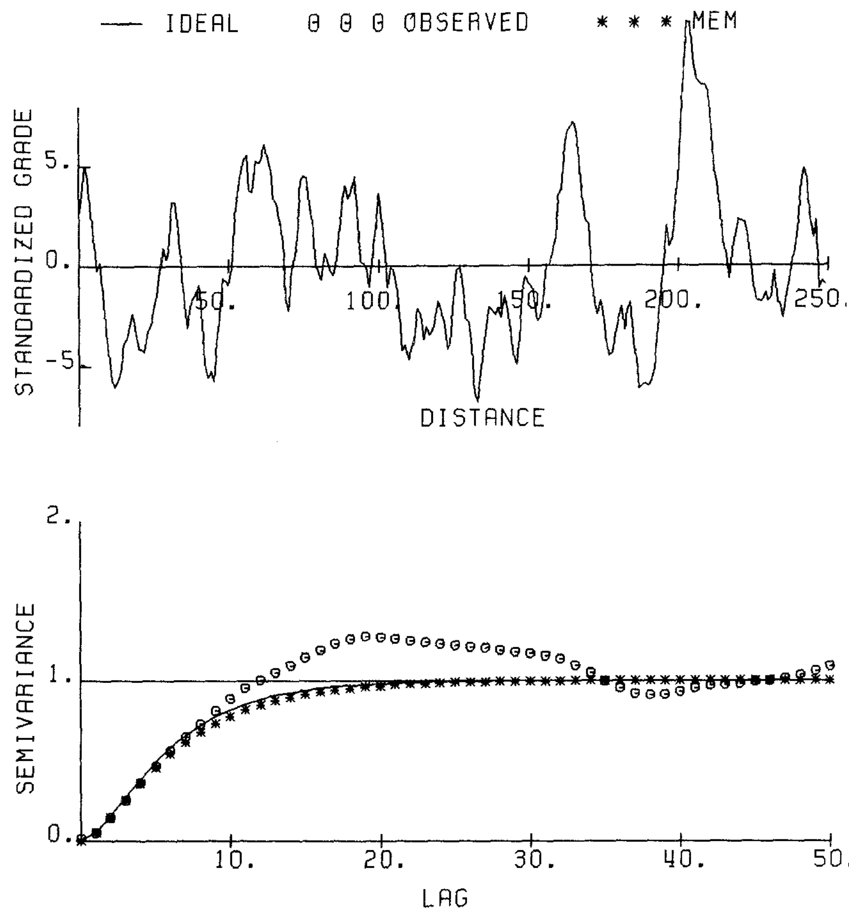

Fig. 4. Ideal, observed, and estimated continuous semivariograms for the ARMA (2 0) process: $g_i = 1.40g_{i-1} - 0.48g_{i-2} + \epsilon_i$. The observed semivariogram was obtained from an artificial series using the generator GGUW and the seed 7822323. The estimated MEM parameters are $\phi_1 = 1.40$ and $\phi_2 = -0.47$.

be interpreted as a first-order AR process, ARMA (1 0), with a superimposed oscillation probably from the instrumentation. The fitted curve yields a $\phi = 0.85$ and except for the undulation agrees quite closely with the observed semivariogram. In the semivariogram of the U analyses (Fig. 7), a similar exponential curvature is found and again the diagram would be interpreted as a first-order AR process, ARMA (1 0). Notice that in the observed series, the very high local values of U have raised the mean above the base level of the series. This

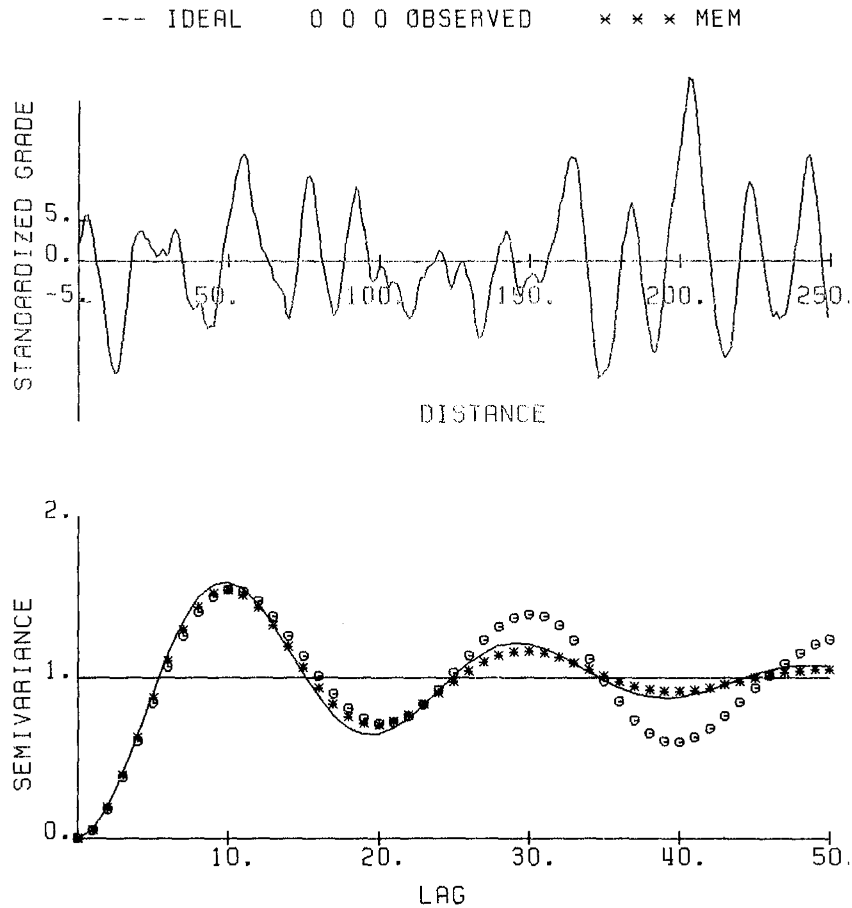

Fig. 5. Ideal, observed, and estimated pseudo-periodic semivariograms for the ARMA (2 0) process: $g_i = 1.80g_{i-1} - 0.90g_{i-2} + \epsilon_i$. The observed semivariogram was obtained from an artificial series using the generator GGUW and the seed 7822323. The estimated MEM parameters are $\phi_1 = 1.79$ and $\phi_2 = -0.88$.

has produced a difference in the sill value between the observed semivariogram and the fitted one ($\phi = 0.90$). The semivariogram of the Th analyses (Fig. 8) shows a marked "hole-effect" and this pseudo-periodic semivariogram is interpreted as a second-order AR process, ARMA (2 0) which yields estimated parameters of $\phi_1 = 1.48$ and $\phi_2 = -0.65$. Notice the excellent agreement between the estimated and observed diagrams at small lags, and then how they wander

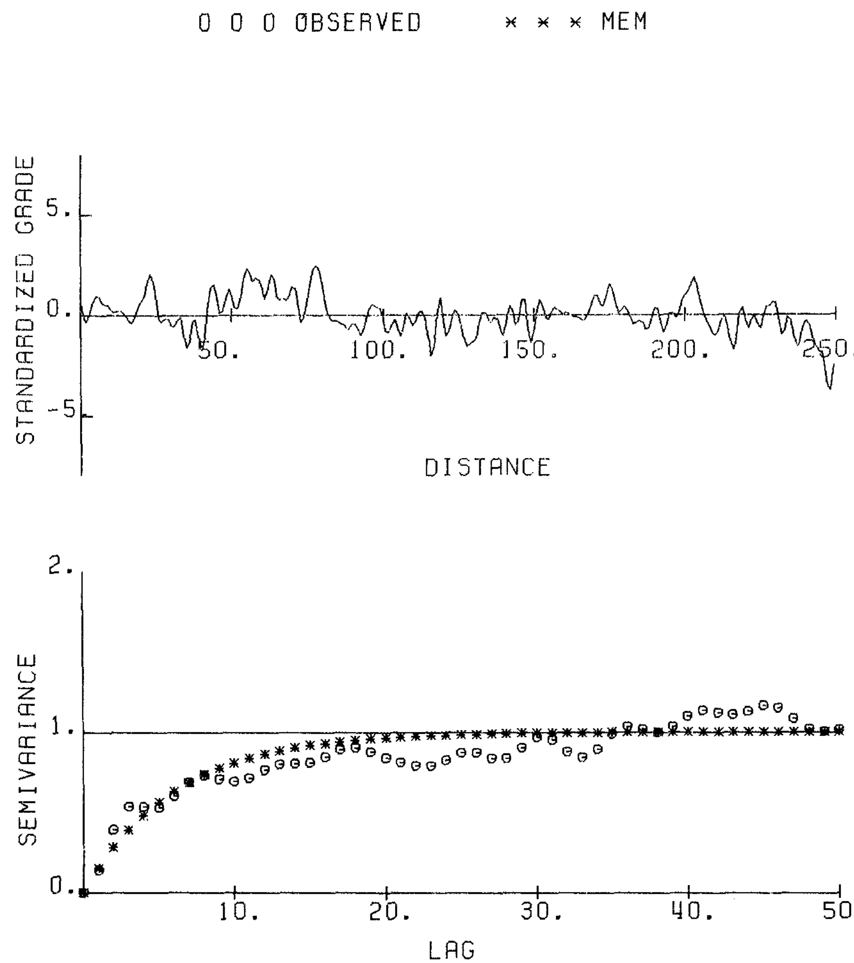

Fig. 6. Observed and estimated semivariograms for a series of K concentrations taken at 0.5-ft intervals from a well log (CM-1) through granite by γ ray spectrometry in the Copper Mountain district, Wyoming. The observed variogram shows exponential curvature with super-imposed undulations. Compare the difference between the observed and estimated (ϕ = 0.85) semivariograms with that found in the simulations (Figs. 1, 2).

away from each other at higher lags in a manner analogous to the simulated case (Fig. 5).

The observations from the Eagle Copper vein at the 6930 level consisted of vein thickness and copper grade (Trimble, 1972). The semivariogram of the vein

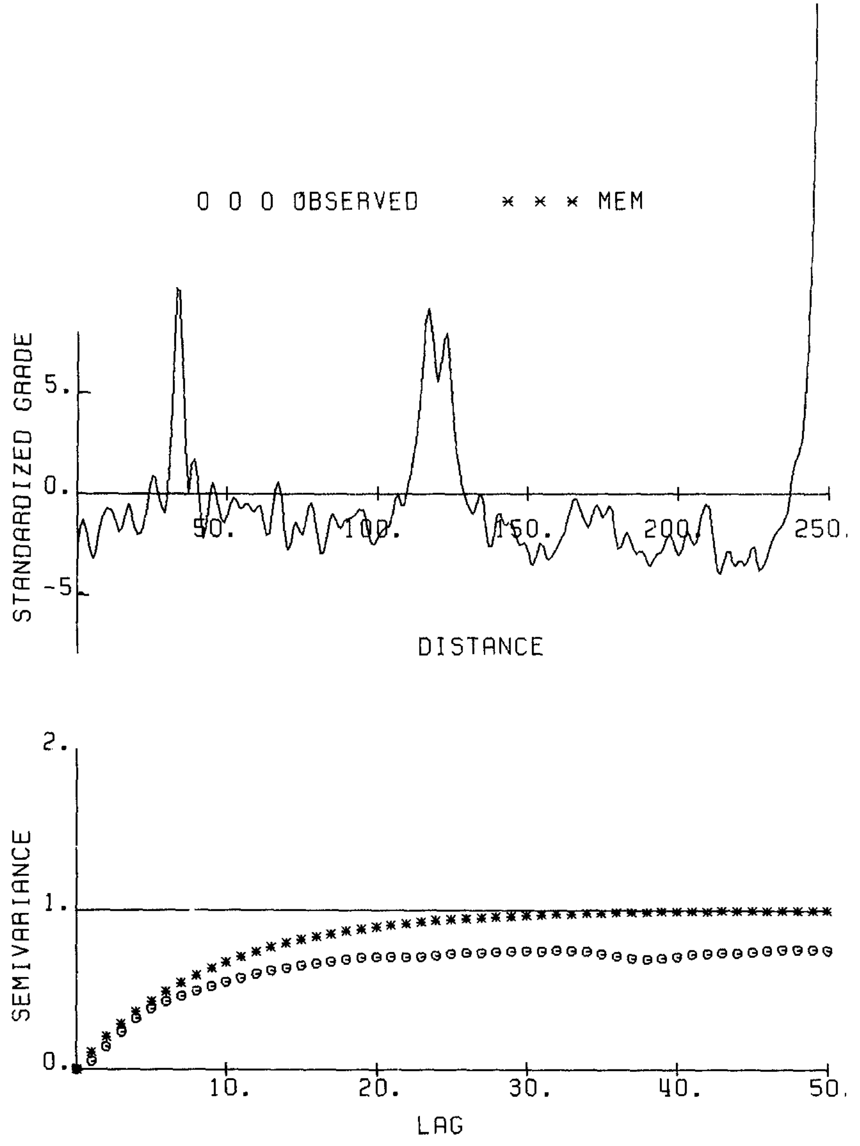

Fig. 7. Observed and estimated semivariograms for a series of U concentrations taken at 0.5-ft intervals from a well log (CM-1) through granite by γ ray spectrometry in the Copper Mountain district, Wyoming. Both variograms show simple exponential curvature but the sill values differ between the observed and estimated ($\phi = 0.90$) because the localized high U values have shifted the mean away from the base values.

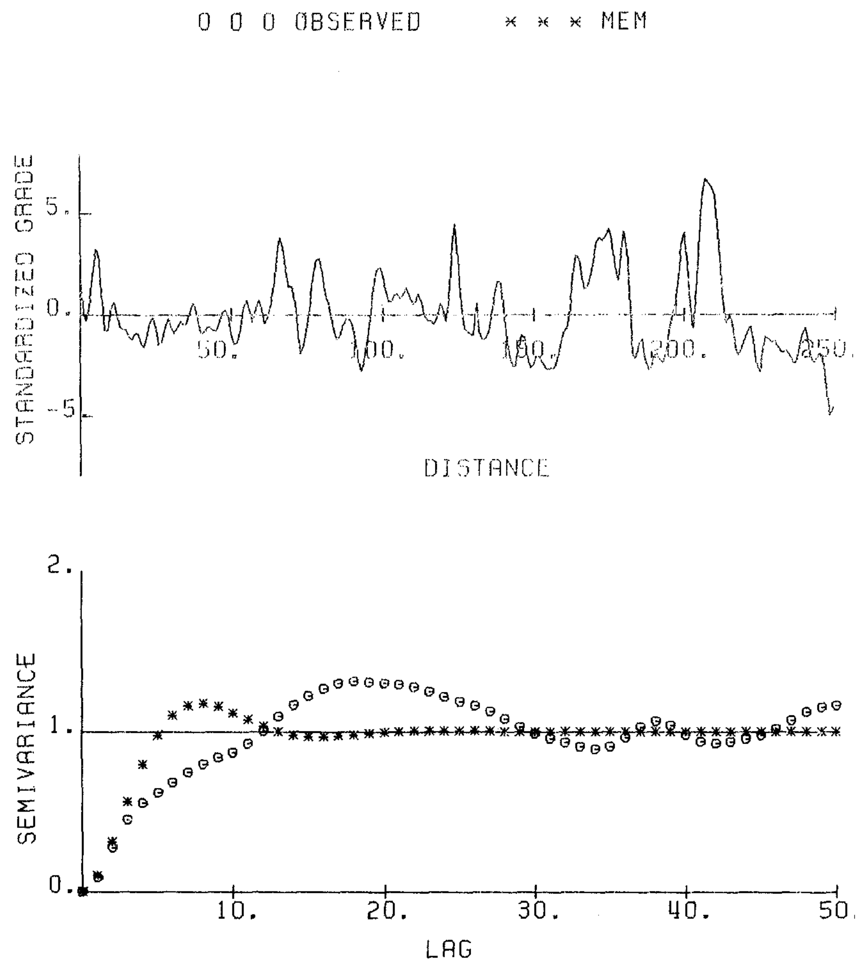

Fig. 8. Observed and estimated semivariograms for a series of Th concentrations taken at 0.5-ft intervals from a well log (CM-1) through granite by γ ray spectrometry in the Copper Mountain district, Wyoming. Both the observed and estimated variograms show a distinct hole effect. Notice the excellent agreement between the observed and estimated ($\phi_1 = 1.48$ and $\phi_2 = -0.65$) variogram at small lags and how they wander apart at intermediate lags.

thickness (Fig. 9) is essentially transitive and has a distinct nugget effect. It may be interpreted as consisting of a first-order AR process with a weighting parameter in the neighborhood of 0.9 combined with a first-order moving average process, ARMA (1 1). Similarly the semivariograms for the copper grade (Fig. 10) and for the accumulation = thickness X grade (Fig. 11) may also be interpreted

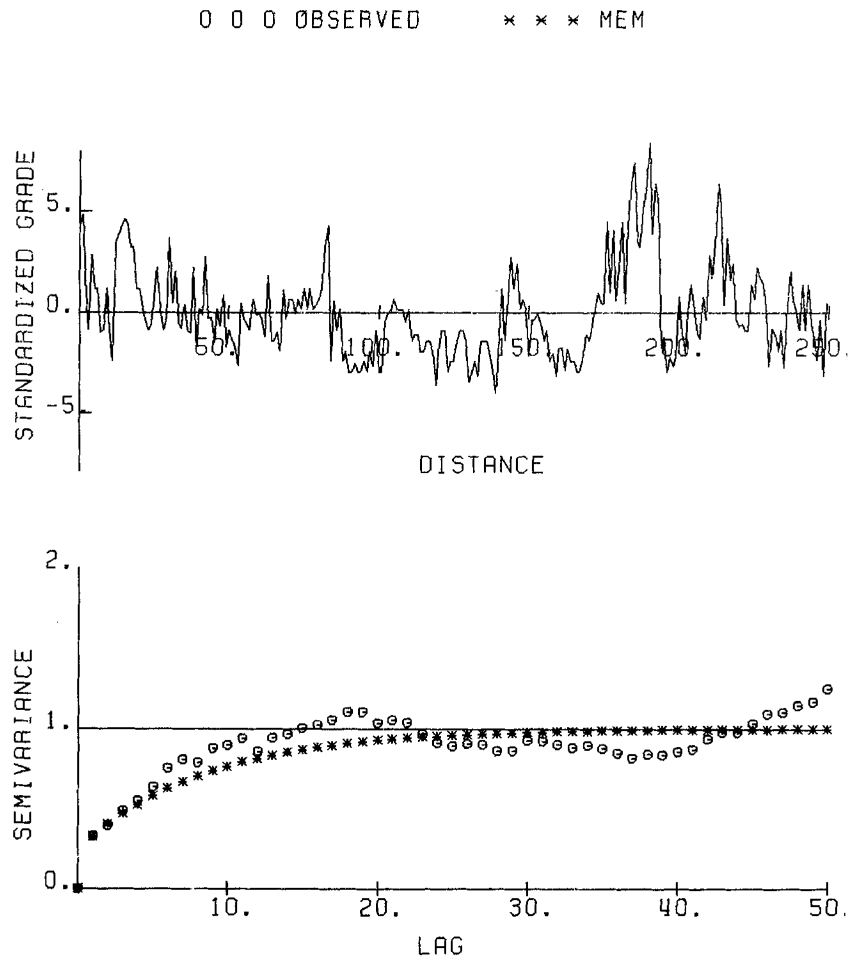

Fig. 9. Observed and estimated semivariograms for a series of vein thicknesses taken at an average interval of 8 ft from the 6930 level of the Eagle Copper vein, British Columbia. Notice how the differences between the observed and estimated (ϕ = 0.87, θ = 0.57) variograms compare to those in the simulated example (Fig. 3).

in the same way but with a larger contribution from the MA process. Notice how the observed and estimated semivariograms of these examples are similar in agreements to that seen between the observed and estimated ones in the simulation (Fig. 3).

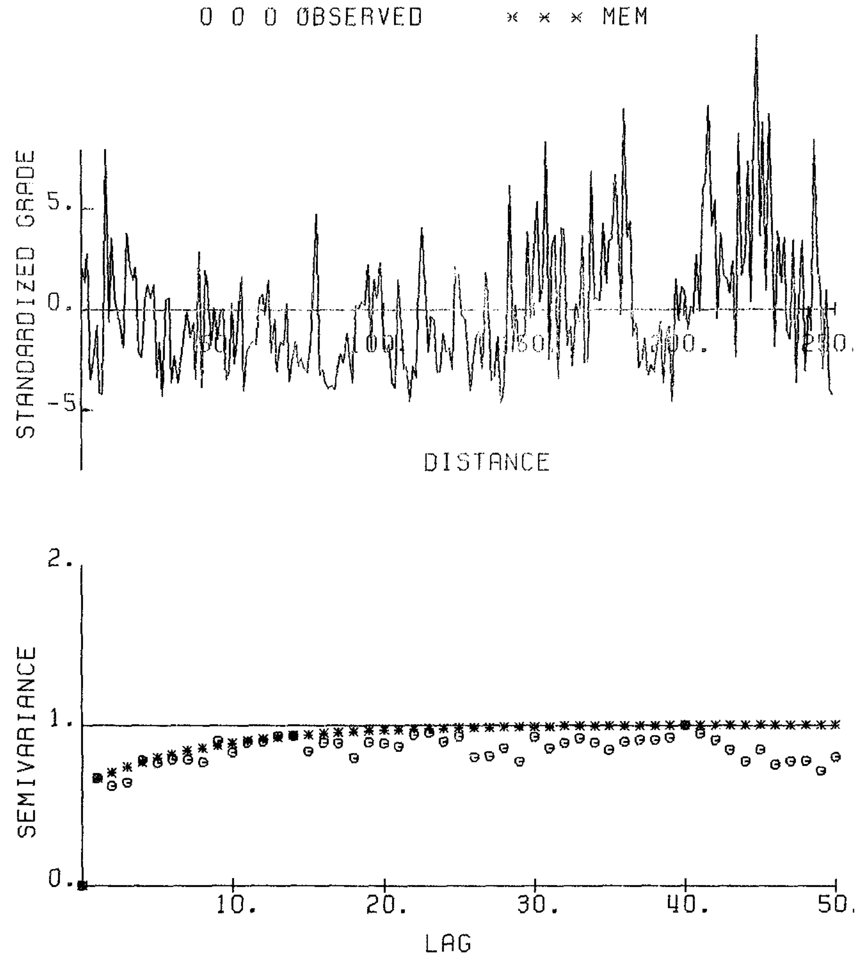

Fig. 10. Observed and estimated semivariograms for a series of copper grades taken at an average interval of 8 ft from the 6930 level of the Eagle Copper vein, British Columbia. The estimated MEM parameters for an ARMA (1 1) process are $\phi = 0.89$ and $\theta = 0.67$.

CONCLUSION

The estimation of the weighting parameters and residual variance using the Burg scheme on computer generated artificial series has proven to be quite effective. However, comparison of the fitted and observed semivariograms may show quite marked departures at intermediate lags; that is between lag 3 and

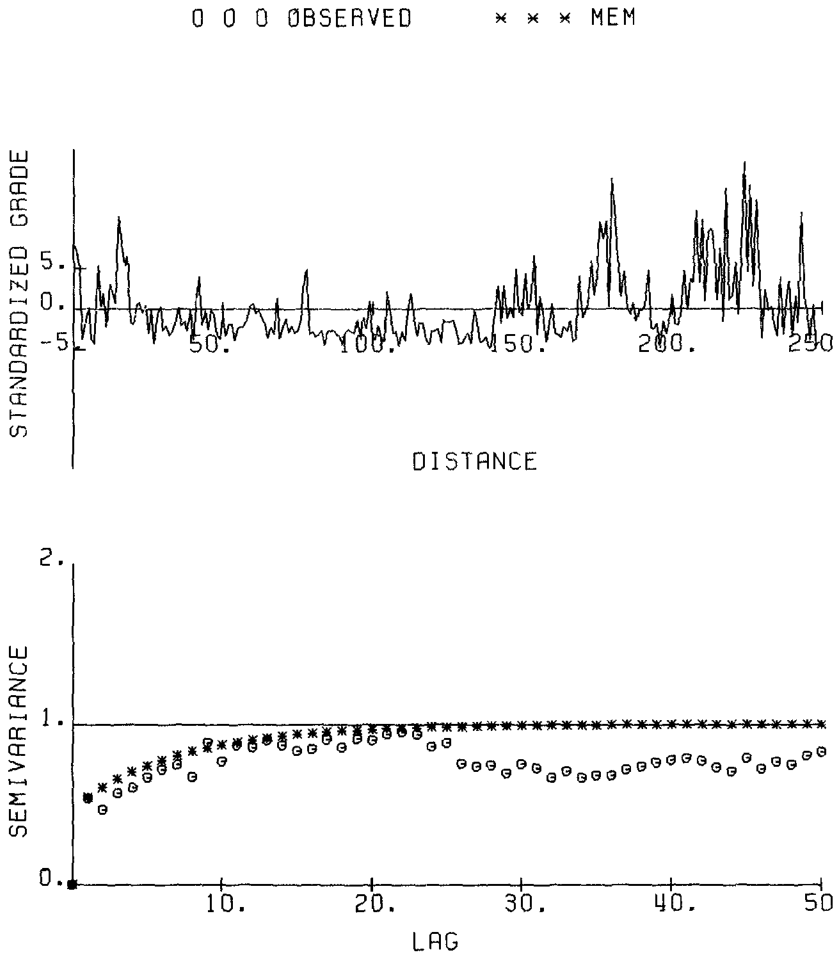

Fig. 11. Observed and estimated semivariograms for a series of accumulations (thickness × copper grade) obtained at an average interval of 8 ft from the 6930 level of the Eagle Copper vein, British Columbia. The estimated MEM parameters are ϕ = 0.87 and θ = 0.57.

the usually accepted range for reaching the sill. This is clearly the result of the finite length of any particular series. This does raise an important consideration regarding the curve fitting of semivariograms as currently practiced and consequently the effectiveness of estimations such as kriging.

There is a natural human tendency and need to fit processes into a long-range scheme in preference to a short range one. This is of course a typical defect in composing stochastic music where it is relatively easy to obtain pieces with pleasant short-range phrases but which tends to wander over longer spans

(Pierce, 1980, p. 259). As a result of this human tendency a good bit of effort has been placed on fitting the long-range curvature of semivariograms. This will, of course, reproduce the original observed series; however, these results can not be expected to apply to any other series, even one a short distance away. This effect has long hampered efforts to make long-range weather forecasts (Panofsky and Brier, 1958, p. 140). Serious attention needs to be given to the relative importance of short- and long-range fitting of semivariograms upon kriging estimates. If the processes being modeled are really stochastic, then temptations to fit the long-range order of any particular series must be ignored and the short-range fit allowed to take precedence.

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REFERENCES

Andersen, N., 1974, On the calculation of filter coefficients for maximum entropy spectral analysis: Geophysics, v. 39, p. 67–72.

Box, G. E. P. and Jenkins, G. M., 1970, Time series analysis, forecasting and control: Holden-Day, San Francisco, 553 pp.

Burg, J. P., 1967, Maximum entropy spectral analysis: presented at the 37th Annual International SEG Meeting, Oklahoma City, October 31, 1967.

Clark, I., 1979, The semivariogram—part 1: Engin. Min. Jour., v. 180 (7), p. 90–94.

Dijkstra, S., 1976, Simple uses of covariograms in geology: Geol. Mijnbouw, v. 55, p. 105–109.

Fuller, W. A., 1976, Introduction to statistical time series: John Wiley & Sons, New York, 470 pp.

IMSL, 1980, IMSL reference manual, 8th ed: International Mathematical and Statistical Libraries, Houston, Texas.

Jowett, G. H., 1955, Sampling properties of local statistics in stationary stochastic series: Biometrika, v. 42, p. 160–169.

Lacoss, R. T., 1971, Data adaptive spectral analysis methods: Geophysics, v. 36, p. 661–675.

Panofsky, H. A. and Brier, G. W., 1958, Some applications of statistics to meteorology: Pennsylvania State University, University Park, Pennsylvania, 224 pp.

Perry, R. and Aroian, L. A., 1979, Of time and the river, time series in *M* dimensions, the one dimensional autoregressive model: Proceedings of the Statistical Computing Section, American Statistical Association, Annual Meeting, p. 383–388.

Pierce, J. R., 1980, An introduction to information theory: Dover, New York, 305 pp.

Ripley, B. D., 1981, Spatial statistics: John Wiley & Sons, New York, 252 pp.

Sharp, W. E., 1981, Stochastic simulation of semivariograms (abstract): American Statistical Association, annual meeting, Detroit, August, 1981.

Taneja, V. S. and Aroian, L. A., 1980, Time series in *M* dimensions, autoregressive models: Commun. Stat., Simul. Comput., v. B9, n. 5, p. 491–513.

Trimble, R. J., 1972, Mineralogy and computer-oriented study of the Eagle vein complex, Liard Mining District, northeastern B.C. (unpublished thesis): Department of Geology, University of British Columbia, 78 pp.

Ulrych, T. J., 1972, Maximum entropy power spectrum of truncated sinusoids: Jour. Geophys. Res., v. 77, p. 1396–1400.