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Variogram Models for Regional Groundwater Geochemical Data[1]

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Four variogram models for regional groundwater geochemical data are presented. These models were developed from an empirical study of the sample variograms for more than 10 elements in groundwaters from two geologic regions in the Plainview quandrangle, Texas. A procedure is given for the estimation of the variogram in the isotropic and anisotropic case. The variograms were found useful for quantifying the differences in spatial variability for elements within a geologic unit and for elements in different geologic units. Additionally, the variogram analysis enables assessment of the assumption of statistical independence of regional samples which is commonly used in many statistical procedures. The estimated variograms are used in computation of kriged estimates for the Plainview quadrangle data. The results indicate that an inverse distance weighting model was superior for prediction than simple kriging with the particular variograms used.

KEY WORDS: variogram, kriging, interpolation, contouring, inverse distance weighting, geochemical gradient.

INTRODUCTION

Many types of geochemical measurements are known to be spatially related. Samples collected from adjacent areas often exhibit a greater degree of dependence than samples collected a greater distance apart. This spatial dependence should also exist for regional hydrogeochemical data. A method for quantifying this dependence is important in understanding regional geochemistry, and is fundamental in the assessment of statistical independence implicit in most traditional data analyses.

Kriging is the geostatistical technique developed by Matheron (1965, 1971, 1973) which focuses on modeling spatial relationships between samples. An important component of the kriging model, discussed in the next section, is the variogram which characterizes the spacial dependency between samples. Most

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uses of kriging have focused on ore reserve estimation (e.g., Journel and Huijbrechts, 1978; and David, 1977) so regional groundwater geochemical data provide a new application area. Burgess and Webster (1980) note several applications in soil mapping over a broad region. Application of variograms to geochemical data was considered by David and Dagbert (1975) over a small region and also by Croissant (1977). The purpose of this study was to develop a variogram estimation procedure and appropriate models for regional groundwater geochemical data. A second objective was to evaluate the simplest form of kriging applied to groundwater data.

The collection of groundwater data as a part of the NURE (National Uranium Resource Evaluation) Program provided an opportunity to explore alternate statistical tools for contouring, anomaly identification, and quantifying spatial dependence. Data from the Plainview National Topographic Map Series (NMTS) quadrangle, Texas (UREP, 1978) were used for this study. Further details may be found in Kane, Begovich, Butz, and Myers (1982) and Myers, Begovich, Butz, and Kane (1980). Other methods of analysis of this data are reported in Beauchamp, Begovich, Kane, and Wolf (1980). (A computer tape of all data can be obtained from Technical Library, Bendix Field Engineering Corp., P.O. Box 1569, Grand Junction, Colorado 81502-1569.)

COMPUTATION OF VARIOGRAMS

Let $Z(x)$ denote the concentration of a geochemical variable at the geographic location x. Consider observations $z(x_i)$ at the n sampling locations $x_1, \ldots, x_n$. An objective of kriging is to estimate the concentrations at unsampled locations or averages over regions. It is assumed that $z(x)$ is a realization of a random function $Z(x)$. The intrinsic hypothesis further assumes that

$$E\{Z(x) - Z(x+r)\} = 0 \tag{1}$$

$$\text{Var}\{Z(x) - Z(x+r)\} = 2\gamma(r) \tag{2}$$

for all vectors x and r. The lack of dependence in (1) on either x or r implies an assumed absence of drift in the variogram $\gamma(r)$. If the variogram depends only on the modulus $|r|$, it is said to be isotropic. However, if consideration of the direction θ is necessary then $\gamma(r) = \gamma(|r|, \theta)$ and the variogram is said to be anisotropic.

If $\text{Var}\{Z(x)\} = K$ is finite and the intrinsic hypothesis is satisfied, then

$$\gamma(r) = \text{Var}\{Z(x)\} - \text{Cov}\{Z(x), Z(x+r)\}, \quad \text{or} \tag{3}$$

$$\gamma(r) = K[1 - \text{Corr}\{Z(x), Z(x+r)\}] \tag{4}$$

As r increases, the behavior of $\gamma(r)$ indicates the value of K. Thus, $\gamma(r)$ is an unscaled reflection of one minus the correlation between two samples a distance r apart.

Since $\gamma(r)$ is in general unknown, it must be estimated from the data. Under the intrinsic hypothesis

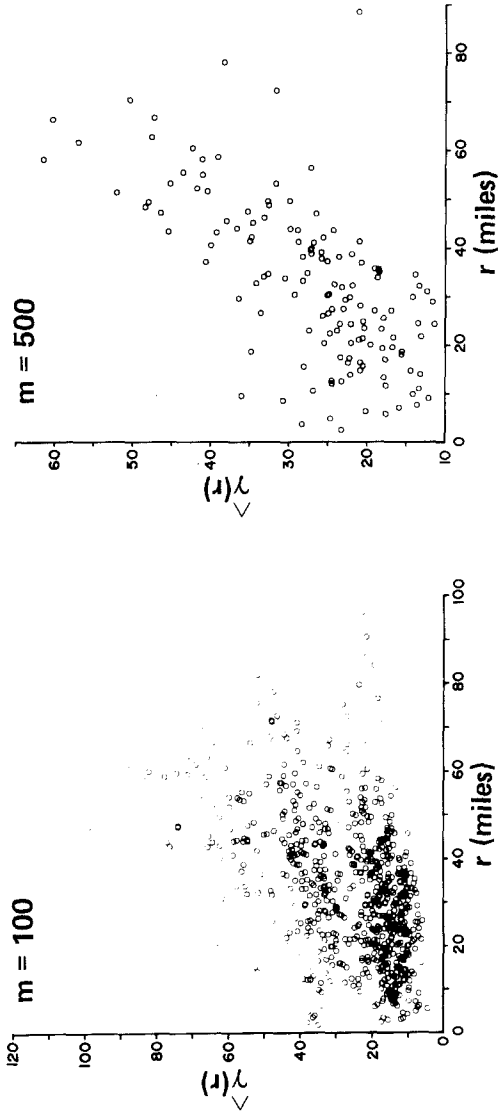
$$\hat{\gamma}(r) = [2(m - 1)]^{-1} \sum [z(x) - z(x + r)]^2 \quad (5)$$

is an unbiased estimator where the summation is over the m pairs of sample locations a distance r apart. The choice of $m - 1$ as opposed to m is simply by analogy with that of the usual unbiased estimator for variance, but for large m it has no real effect and either may be used. The quantity $\hat{\gamma}(r)$ is an estimator of the value of $\gamma(r)$ for each r and is not an estimator of the variogram model since in general $-\hat{\gamma}(r)$ is not conditionally positive definite. The computation of $\hat{\gamma}(r)$ for regional groundwater geochemical applications presents several problems.

The intrinsic hypothesis implicitly assumes a common geologic population and this may be difficult to satisfy for regional applications. (As will be noted later, the fitting of the variogram model utilized $\hat{\gamma}(r)$ only for r less than 30 and the kriging utilized only sample locations within 10 miles, hence the intrinsic hypothesis was used only locally.) For example, the Plainview quadrangle contains two major geologic environments, the Ogallala formation and the Permian units. The example variograms in the next section illustrate the differences in the environments. Further division of the Permain units was examined by Beauchamp, Begovich, Kane, and Wolf (1980), but no significant differences in the variograms could be detected. However, the partitioning of samples by geologic strata increases the variability of $\hat{\gamma}(r)$ since the samples sizes are reduced.

A second problem in computation of $\hat{\gamma}(r)$ is that regional groundwater geochemical sampling is often not conducted on a fixed grid as in mining applications, but is typically irregular. Although the grid was not uniform there was no clustering and intersample distances were on the order of 3.5 miles. Thus, m in (5) would be small for a particular r even with the large sample sizes as in the Ogallala formation ($n = 357$) and Permian units ($n = 471$). To reduce variability, the observed distances between samples were grouped into variable length intervals. The interval size was determined so that a constant number of sample pairs were in each interval. The mean r was then used for the interval. This procedure results in each plotted point on the variogram being computed from the same sample size. Figure 1 illustrates the sensitivity of $\hat{\gamma}(r)$ to changing m. Only at $m = 1000$ was a consistent pattern discernable. In particular for $m = 100$ there is so much scatter that the plot has no discernable shape at all. Thus $m = 1000$ was used for the remainder of the computations except where otherwise noted.

Another difficulty in the variogram computations is the determination of the appropriate scale in which to express $Z(x)$. The original scale of measurement is preferable. However, the intrinsic hypothesis may be more appropriate in a transformed scale. For example, ignoring spatial relationships, geochemical data are often considered lognormally distributed which implies that the mean


m = 500
m = 100
r (miles)
r (miles)
γ(r)
γ(r)

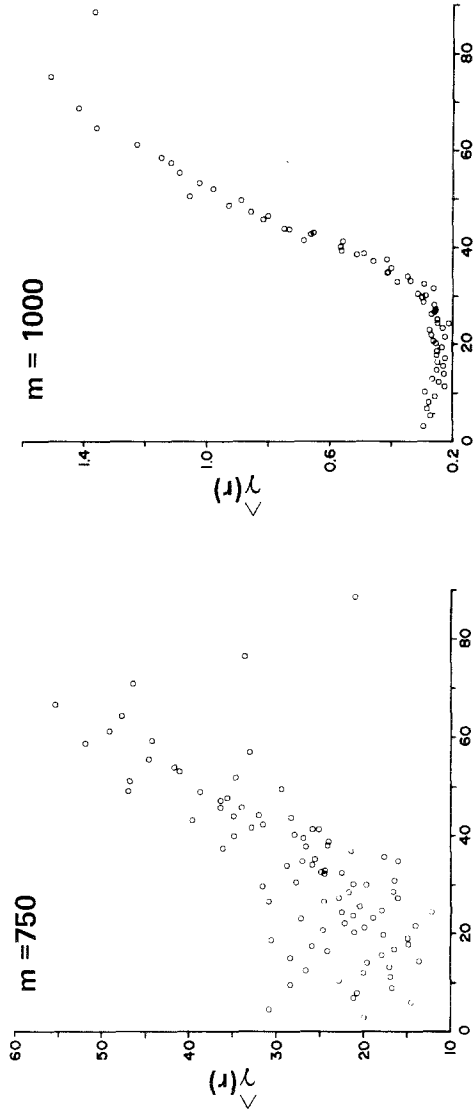
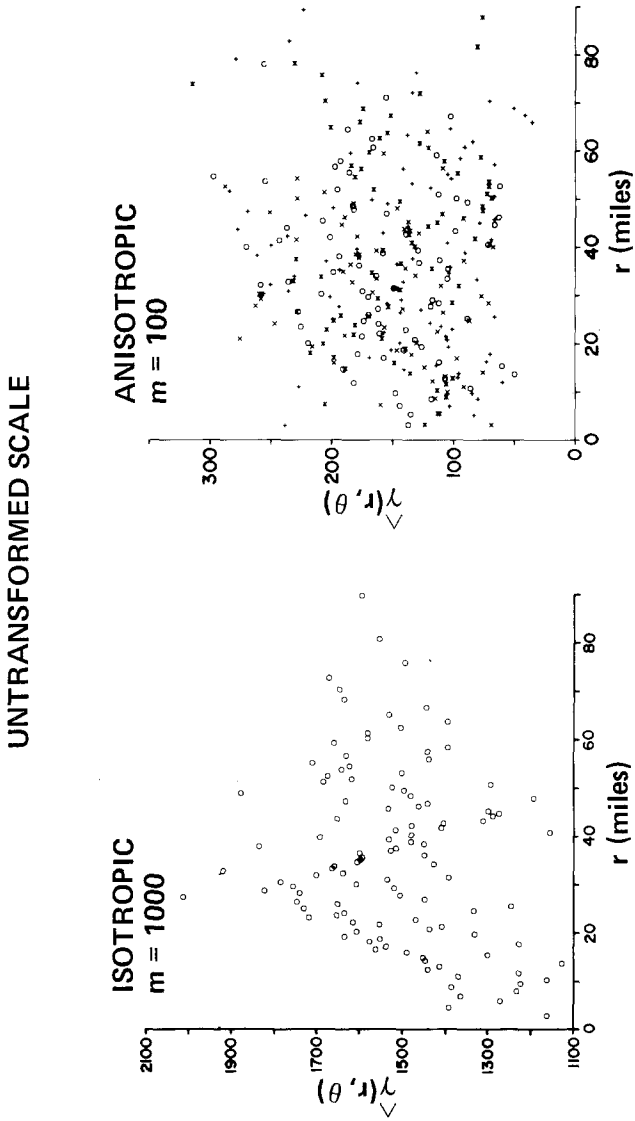


Fig. 1. Isotropic variograms for uranium in the ogallala formation using a varying number of points per interval.


UNTRANSFORMED SCALE
ISOTROPIC
m = 1000
ANISOTROPIC
m = 100
$\hat{\gamma}(r, \theta)$
r (miles)
2100
1900
1700
1500
1300
1100
300
200
100
0
0
20
40
60
80

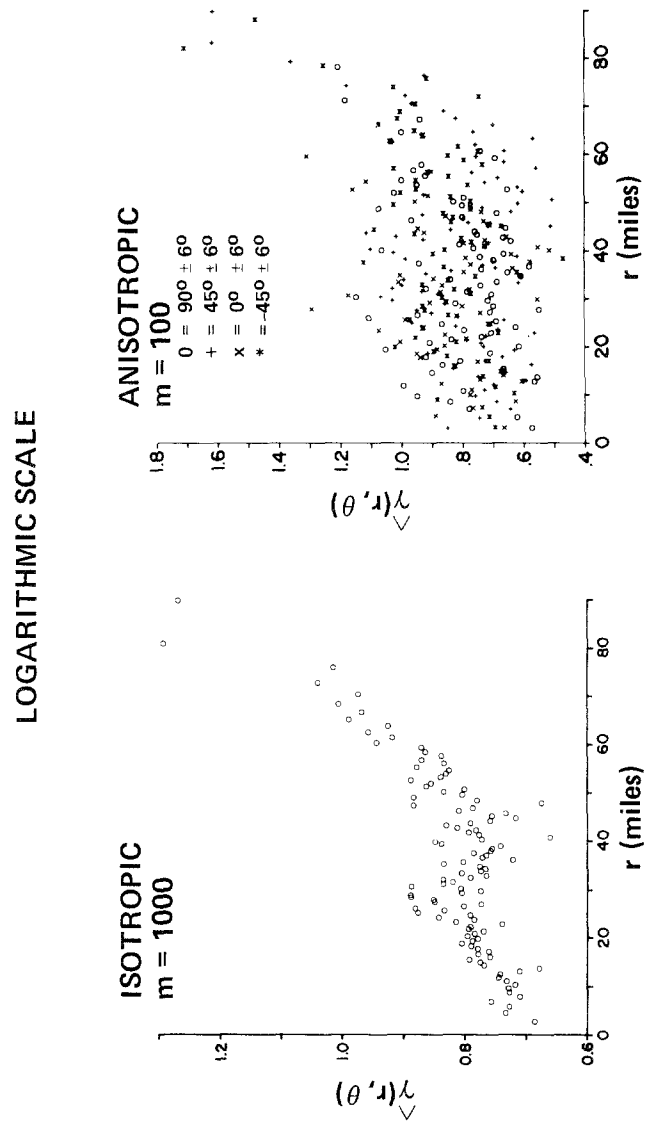


Fig. 2. Variograms for uranium in the Permian units.

of $Z(x)$ depends on the variance of $\ln Z(x)$. Thus, computation of $\hat{\gamma}(r)$ may be more appropriate for $\ln Z(x)$. The major difficulty in using $\ln Z(x)$ is that biased predictions of $Z(x)$ are obtained from the kriging estimation procedure. Fig. 2a, c gives the untransformed and logarithmic isotropic variograms for uranium in the Permian units. Notice that there is no discernable pattern in the untransformed scale.

Anisotropic variograms were computed by the same procedure as the isotropic variograms, but only samples within a specified direction were considered. If no anisotropies exist, the anisotropic variograms for specified angles should appear the same as the isotropic variograms. Unfortunately, considering only samples within the specified angles appreciably reduces the number of available sample pairs. As was seen from Fig. 1, this limits the usefulness of the estimated variogram. Fig. 2b, d gives anisotropic variograms for $m = 100$ for uranium in the Permian units. No anisotropies were detected in either the Ogallala formation or Permian units.

VARIOGRAM MODELS

The variables chosen for analysis were selected to allow characterization of major as well as trace element geochemistry and are restricted to those variables where a sufficient number of samples are above the laboratory detection limit for measurement. Estimates of the isotropic variogram were computed for the 13 variables U, B, Ba, Ca, Li, Mg, Mo, As, V, SO_4, Specific Conductance (SCON), the total alkalinity (ALK) in the Ogallala formation, and the same 12 variables in the Permian units with As omitted because of a limited range of values. Examples of typical sample variograms appear in Fig. 3.

A method of interpreting the sample variograms is simply to group them by apparent similarities. Figure 4 indicates the apparent graphical forms observed. These could be modeled by functions of the following form

$$g(r) = \begin{cases} 0 & r \leqslant 0 \\ \alpha & 0 < r \leqslant a \\ \alpha + \beta r^{\lambda} & a < r \leqslant b \end{cases} \tag{6}$$

For $a > 0$, $g(r)$ is not a valid variogram model since $-g(r)$ is not necessarily conditionally positive definite. It was necessary to alter (6) to obtain a valid estimator of the variogram. Although the constant linear model is graphically descriptive of some sample variograms, it may be that the model should be parabolic, which would be indicative of drift. It may also be that this shape is a consequence of the smoothing that results from using $m = 1000$. The results of the graphical classification and are discussed in the next section.

The models in Fig. 4 could be interpreted in terms of (4). In that case, the

linear model simply implies that the correlation between pairs points decreases constantly with increasing distance. The constant-linear model implies that there is an initial distance in which the correlation is constant followed by a decreasing correlation. The concave (convex) model implies that the correlation decreases at a decreasing (increasing) rate with increasing distance between samples. As will be seen, these models can be useful in the interpretation of regional groundwater data.

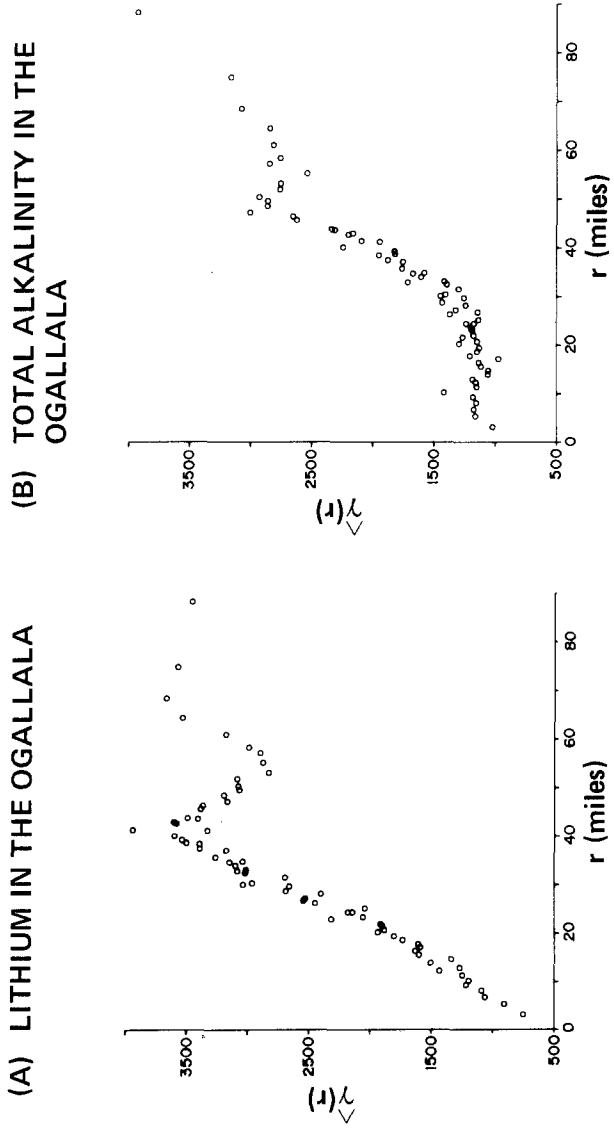
Several features of the sample variograms for the groundwater data are different than typical mining variograms. A sill where the variogram becomes level as r increases was not apparent or it exists only for much greater distances. When there is no sill, it is important to consider the growth of $\gamma(r)$. Journel and Huijbrechts (1978, p. 39) note that this intrinsic hypothesis implies

$$\lim_{|r|\to\infty} \frac{\gamma(r)}{|r|^2} = 0 \tag{7}$$

Thus, the models in Fig. 4 imply that a sill exists, but may not be present over the observable range of r.

Another characteristic of the sample variograms was that a "nugget effect" (i.e., nonzero intercept) was always present for both major and trace elements. In mining applications, the discontinuity at the origin may be caused by irregular mineralization due to small high-grade accumulations. For regional groundwater data, rapid changes over a very short distance within the same geologic unit seem unlikely. Possible explanations for the observed nugget effect include: (1) Very little data was available for small r since the sample grid was 3.2 miles (5.1 km). (2) The changes in concentration are large relative to the scale of sampling. (3) The intrinsic hypothesis was not appropriate and a more complex kriging model is necessary. (4) The true variogram is not a generally smooth function near $r = 0$ and does intersect the origin, but increases quickly for $r > 0$.

In order to utilize kriging, it is necessary to fit an acceptable functional model so that $-\hat{\gamma}(r)$ is conditionally positive definite. For this purpose, models of the sample variogram, $\hat{\gamma}(r)$, were considered of the form $\gamma(r) = \alpha + \beta r^{\lambda}$ where λ was assumed fixed at $\lambda = 1$, 0.5, or 1.5. The coefficients α and β were chosen by a least squares fit. Although sample variograms were computed and plotted for up to 90 miles, the number of pairs diminishes rapidly beyond 30 miles and the models were fitted only for the first 30 miles. Thus, the constant-linear model resulted in $\hat{\beta}$ close to zero. Subsequently, data locations within 10 miles were used in the kriging. Increasing r appreciably increases the computational time since an increasing number of samples are being used for the kriging estimation. The R^2 measure from least squares (one minus the residual sum of squares divided by the corrected total sum of squares) is given in Table 1 along with S values that are discussed in the next section.


(A) LITHIUM IN THE OGALLALA
(B) TOTAL ALKALINITY IN THE OGALLALA
γ(r)
r (miles)
0
20
40
60
80
500
1500
2500
3500

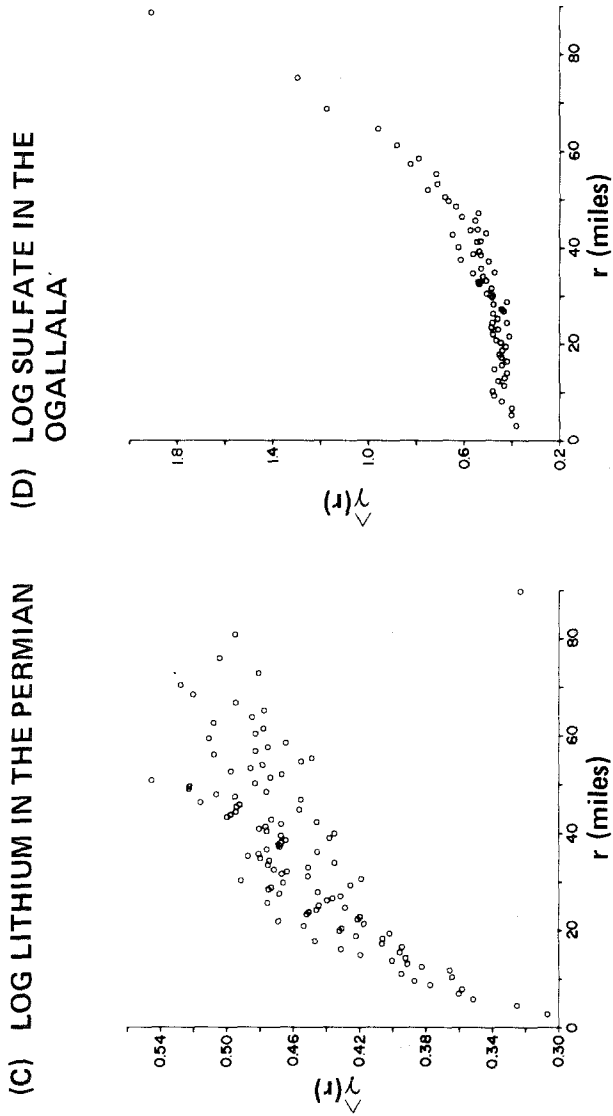


Fig. 3. Example variograms from the plainview quadrangle.

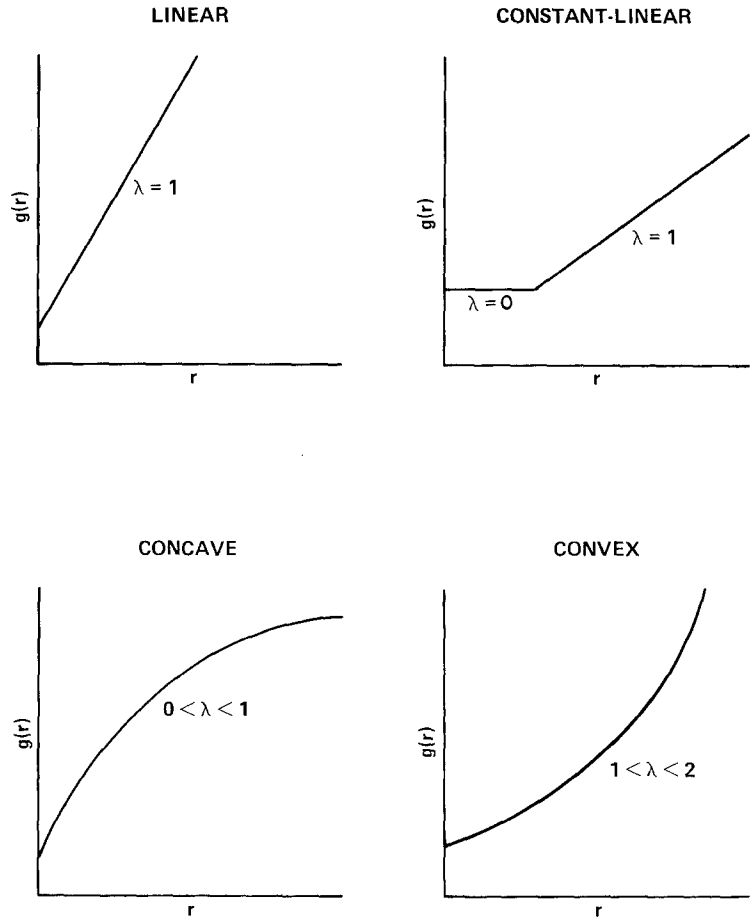


Fig. 4. Variograms models for regional geochemical data.

INTERPRETATION OF PLAINVIEW DATA

The sample variograms provide several types of useful information. Within a geologic unit, variograms quantify the spacial correlation exhibited by elements and the "sharpness" of geochemical gradients. The constant-linear model indicates that out to some distance (a) variation is constant. The linear, convex, and concave models indicate an increase in variation with distance. This implies that elements which fit the constant-linear model should have a more homogeneous distribution relative to elements fitting other models. As an example, a contour map of uranium (constant-linear variogram) in the Ogallala formation is much more uniform than a map of molybdenum (linear).

Table 1. Summary of Results from Plainview Quadrangle Analyses

Element	Ogallala[a]			Permian[a]		
	R^2	S_K	S_I	R^2	S_K	S_I
U	0.10	2.03	1.20	–	–	–
ln (U)	0.56	1.81	1.28	0.25	0.99	0.86
SCON	0.15	1.59	0.90	0.29	0.66	0.71
ln (SCON)	0.69	0.93	0.74	0.63	0.78	0.77
B	0.21	1.56	1.12	–	–	–
ln (B)	0.78	1.26	0.84	0.04	0.95	0.89
Ba	0.71	–	1.11	0.07	4.11	0.86
ln (Ba)	0.57	1.29	1.03	0.39	0.94	0.77
Ca	0.04	4.24	1.38	0.75	0.81	0.82
ln (Ca)	0.30	2.18	1.35	0.57	1.26	0.76
Li	0.98	0.43	0.41	0.58	0.78	0.64
ln (Li)	0.95	0.88	0.49	0.74	0.58	0.54
Mg	0.34	3.96	0.72	0.18	0.96	1.00
ln (Mg)	0.60	2.12	1.10	0.35	0.92	0.91
Na	0.43	2.91	1.21	–	–	–
ln (Na)	0.69	1.56	1.08	0.27	0.75	0.72
Mo	0.17	20.1	4.25	–	–	–
ln (Mo)	–	–	–	0.12	1.20	0.87
SO_4	–	–	–	–	–	0.88
ln (SO_4)	0.58	0.81	0.75	–	–	0.63
ALK	0.71	1.32	0.73	0.81	0.78	0.67
ln (ALK)	0.49	1.04	0.67	–	–	0.56
V	–	–	–	–	–	–
ln (V)	0.93	0.83	0.72	0.11	1.20	0.98
AS	0.69	0.84	0.81			
ln (AS)	0.88	1.00	0.86			

[a]A dash indicates that no analysis was performed.

Families of elements can be grouped together that fit types of models to establish their similarity and conclusions drawn concerning the relationships. For example, uranium, boron, barium, calcium, magnesium, sodium, and alkalinity fit the constant-linear model. The distribution pattern of uranium fits that of several major elements in terms of wide homogeneous distribution. Molybdenum, arsenic, and vandium, which fit the linear model, have sharp local gradients and may be very useful as pathfinder elements to identify those

areas of interest containing high concentrations of uranium among the broad uranium trends.

Between geologic units variograms can demonstrate relative differences in behavior of elements in different groundwater geochemical systems and suggest the scale of future sampling. In the Ogallala formation, uranium fits the constant-linear model while in the Permian units uranium is linear. This implies different controls on uranium distribution in the Permian units which result in relatively sharper gradients and a less homogeneous distribution. Many of the elements fitting the constant-linear model in the Ogallala formation fit a linear model in the Permian units. In fact, there are fundamental differences in geochemical controls between the units and this is reflected in the variogram models. A further comparison between the same element in the two different units indicates that the variogram models can be used to define the relative scale of sampling necessary to characterize elemental distributions based on the model type. The variation of uranium in the Ogallala formation is constant for sample spacings of up to 30 miles while in the Permian Units variation increases constantly. One could use this information in designing a subsequent sampling plan to conclude that in looking for uranium, the sample spacing in the Ogallala formation could be much greater than in the Permian units to arrive at an equally representative distribution map.

Once functional models are fitted to the sample variograms, it is possible to apply the standard kriging estimation. The Plainview quadrangle data was used to evaluate Kriging relative to an optimal inverse distance weighting (IDW) procedure discussed in Kane, Begovich, Butz, and Myers (1981). A useful method of comparison of two estimation procedures is using the statistic

$$S = \frac{\sum_{i=1}^{n'} (z_i - \hat{z}_i)^2}{\sum_{i=1}^{n'} (z_i - \bar{z})^2} \tag{8}$$

where $\hat{z}_i$ is the estimated value of z_i for $i = 1, \ldots, n'$ validation sample locations (Kane, Begovich, Butz, and Myers, 1981). This is a form of jackknifing and the numerator represents a comparison between the observed value at the ith location and the kriged value using only nearby sample locations, namely within 10 miles. For some sample locations as few as 9 other sample values were used in the estimation, for others as many as 40. In the first stage of the project only punctual kriging was used and it is likely that block kriging would provide improved comparisons for kriging. It had been intended to pursue this in subsequent work. It should be noted that for $S > 1$ it is on the average better to replace estimated values by the sample mean ($\bar{z}$). Thus if $S > 1$, the usefulness of an estimation method may be limited for interpolation at unsampled points.

It was found in some instances that the value of S was very sensitive to the inclusion or deletion of a small number of points. Other forms of S were considered whereby the differences were normalized by the estimation standard deviation or by the deletion of points where the differences exceeded two standard deviations. Histograms of $z_i - \hat{z}_i$ were plotted both for kriging and IDW which provided evidence that the estimators were unbiased.

The values of S for kriging (S_K) and IDW (S_I) appear in Table 1 for the Plainview data. For many of the variables S_K was larger than S_I, which would suggest that IDW was a better estimator than kriging for the optimal choice of the exponent in the IDW and the particular variogram models used. The deficiency of the kriging estimator in these cases may also be due to the presence of drift which was not accounted for, that is, universal kriging was not used. Journel and Huijbrechts (1978, p. 40) note from (7) that variograms that increase faster than $|r|^2$ indicate the presence of drift [i.e., $E\{Z(x)\} = M(x)$]. Several rapidly increasing variograms were noted in the Plainview data. It should be noted that cases where kriging estimation was generally useful correspond to large R^2 values (e.g., Li and total alkalinity). Thus, the absence of a large component of random variation (i.e., large R^2) in the sample variogram justifies the underlying assumptions and then kriging is applicable.

The discrepancies between IDW and kriging may be utilized in another way. One of the objectives discussed in Myers, Begovich, Butz, and Kane (1980) is the identification of anomalous or unusual sampling locations. One method of identifying unusual locations is by scaling the residuals $\hat{z}_i - z_i$ in terms of the estimation standard deviation. In many instances, it was found that the large S values was due to a large number of unusual points. In terms of a strict stationary assumption, some of these points would be considered outliers and could have an effect on variogram estimation, but this effect is substantially ameliorated by using $m = 1000$.

CONCLUSIONS

Four types of variogram models were used to fit the groundwater sample variograms. A single functional form can be used to estimate the variogram. Several factors were noted from the Plainview Quadrangle sample variograms: (1) Many elements exhibited a "nugget effect" and the absence of a sill. (2) The constant-linear variogram model was prevalent in the Ogallala with a constant range of 30 miles. (3) Sample variograms differed appreciably between both geochemical variables and geologic units. Variograms were shown to reflect differences in elemental spatial correlation both within and between geologic units. The sample variograms quantify geochemical gradients enabling useful interpretations of groundwater data and suggesting follow-up sample spacing. Future applications of kriging should entertain more complicated models, such as the

incorporation of drift, since several sample variograms exhibited appreciable scatter and kriging estimates of sample points were often inferior to the IDW estimates.

ACKNOWLEDGMENTS

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