GEOSTATISTICAL ASSESSMENT OF THE SPATIAL VARIABILITY OF SOIL NITRATE IN AN AGRICULTURAL FIELD

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LITERATURE REVIEW

Conventional soil sampling techniques employ a method of random selection in which the relationship between samples is not considered. Each sample removed from a field is independent, and the variability between that sample and neighboring samples is usually not examined. Samples are usually averaged, providing a mean for a field or area of interest, a value that may not adequately describe the behavior of the nutrient across the area of interest. By contrast, geostatistical techniques explore spatial relationships between samples, examining the changes in sample values over both distance and direction.

Relatively new methods for assessing the spatial variability of soil characteristics are the geostatistical techniques of variogram construction, coupled with the estimation of values by kriging. Variogram construction provides an illustration of the behavior of the soil characteristic across a field, while kriging estimates unknown values within and, possibly, beyond the site. Variograms and kriging are not the only geostatistical procedures for describing variability and estimating values, but they are two commonly found in the soil science literature.

Variograms can be constructed from many types of data sets, and the technique is adaptable to different soil characteristics and sampling schemes.

The general equation for variogram calculation is:

$$\boxed{\gamma(h) = \frac{1}{2N} \sum \left(x - (x+h)\right)^2}$$

where: x = variable at location x
h = distance between samples (lag distance)
(Journel and Huijbregts, 1978)

This equation may be modified (Cressie and Hawkins,1980; Cressie, 1985), but the basic procedure of squaring the difference between two values usually remains.

Variograms are usually shown as line diagrams, with the variogram value at a given lag (g(h)) plotted against that lag distance, h. The "one-half" term in the equation divides the symmetrical curve of the variogram in half, so that the plotted information is most accurately called a semivariogram. Semivariograms can be created both omnidirectionally and directionally. Omnidirectional semivariograms offer an initial picture of spatial variability--a preview of possible complications that may arise within directional semivariograms. Directional variograms illustrate variations in spatial relationship as the sampling direction changes across the site.

Variograms are created from available data points, and a model is fit to this experimental variogram. The model is often initially fit to an omnidirectional semivariogram, providing the best fit to a smooth "average" semivariogram. Directional semivariograms are then used to indicate the presence of anisotropies, where spatial relationships differ over various directions. The presence of anisotropies can affect the accuracy of models fit to the semivariogram, which will in turn alter the kriging estimates.

A modeled variogram provides several pieces of information about the sampled site. First, the model can supply an estimate of the nugget, that portion of the semivariogram attributable to pure random error. Second, some models will estimate the sill, where the semivariogram may level. Third, the distance at which samples are no longer spatially related to each other can be found. This distance is called the range. Figure 1 (p. 11) illustrates a typical variogram shape, with the nugget, sill, and range marked by a,b, and c, respectively.

The choice of the model and the accuracy of the model's fit to the semivariogram is important, as the coefficients derived from the model are used in the estimation procedure of kriging. Kriging calculates estimates using weighted linear combinations of available data. It is both an unbiased and best estimation method in that kriging attempts to have the mean error equal zero and the variance of these errors minimized (Isaaks and Srivastava, 1989). Kriging can be used to estimate an unknown point, as with ordinary kriging, or the kriging procedure may be modified to provide an average estimate for a small local area of interest, a technique called block kriging. This paper will use block kriging to produce average estimated values throughout the sampled agricultural site.

Detailed and informative discussions about the theories and methodologies of semivariogram construction and kriging can be found in many sources, including Isaaks and Srivastava (1989); Journel and Huijbregts (1978); Hamlett, Horton, and Cressie (1986); and Warrick and Myers (1987).

The soil science literature that examines the spatial variability of soil characteristics is relatively small and new, though increasing rapidly. Geostatistical techniques were first developed for estimating the depth and size of ore reserves, and the theories were not widely available until Matheron's (1963) publication. The methods then began to make their way from mining into other research areas, including soil science.

Often, soil scientists used semivariogram construction to study the spatial variation of soil physical properties. Among these properties were sand content (Campbell, 1978; Tabor,1985; Nash,1988), infiltration rate (Vieria,1981) and soil-water pressure potential (Hamlett,1986). Other examined physical properties include clay content (Tabor,1985;

Nash,1988; Ovalles and Collins,1988), soil temperature (Mulla,1988; Yates,1988), depth to mottles (Di,1989) and soil heat flux (Wolf and Rogowski, 1991).

Analyses of soil chemical properties through the use of geostatistics have centered upon properties such as pH (Campbell,1978; Tabor,1985; Laslett and McBratney, 1990) and organic carbon content (Ovalles and Collins, 1988; West,1989). Fewer papers have explored the spatial variability of fertility nutrients such as phosphorus, potassium and nitrogen (Tabor,1985; West,1989). In these studies measured K was as the exchangeable form, while analyzed P content was either Total or extractable P. The form of N that was examined varied, including Total-N (West,1989), solution-NO3 (Flaig,1986), petiole-N, and nitrate-N (Tabor,1985).

Although the creation of semivariograms is a fairly standard technique, data sets are sometimes manipulated prior to semivariogram construction. Transformations included a logarithmic conversion, creating soil nitrate and phosphorus data that followed a normal distribution (Tabor, 1985), and a logarithmic conversion followed by median subtraction, removing trend in a soil-water tension data set (Hamlett, 1986). By comparison, surface measurements of extractable P, exchangeable K, and Total N were employed in semivariogram construction without initial transformations (West, 1989).

As an estimation process, kriging of soil characteristics produced varying degrees of success. Point kriging of CaCO3, clay, and sand found promise as an estimation method, but dense sampling would be needed to lessen large nugget effects (Nash,1988). In another paper, kriged values of extractable P, exchangeable K, total N, and organic C from grazed pastures estimated zones of accumulated P and K near drinking water sources. It was felt that kriging could illustrate zones of nutrient enhancement that could be sampled separately for more effective fertilizer recommendations (West,1989). Estimation of field-measured infiltration rates by kriging provided a mean estimation error that was close to zero, coupled with a low variance of the estimation errors (Vieria,1981). A small mean estimation error and a low variance of the estimation errors indicates reliable kriged estimates.

Block kriging is often found to provide more accurate estimates, when that procedure is compared to punctual kriging. Estimated sodium content from block kriging contained much lower estimation variances than sodium contents estimated by punctual kriging (Burgess and Webster,1980). Block kriging was used to estimate electrical conductivity (ECe) and soil nitrate (Tabor, 1985). It was found that soil nitrate was well correlated with ECe, exhibiting similar spatial structure over the sampled site. The kriging error variance was small, indicating that the block kriging procedure was estimating unknown values well.

The spatial variability of soil nitrate remains largely undocumented. The spatial variability of nitrate might be large, a function of large fluctuations in soil nitrate content, or, by contrast, the spatial variation of soil nitrate may decrease as this mobile form of N is removed (Biggar,1978). An examination of the spatial structure of soil nitrate both horizontally and vertically in a field may provide a clearer picture of the spatial behavior of this mobile nutrient. The need for the spatial description and estimation of soil nitrate values is both economic and environmental. Identifying the degree and type of spatial relationships that exist for soil nitrate may help increase the accuracy of soil sampling and testing, affecting the quantity and placement of fertilizer and lime applications. Additionally, the estimation of nitrate values at unsampled regions may place focus upon areas of the field that contain higher levels of nitrate, areas that contain the potential for nitrate leaching to occur. The objective of this research project was to describe the spatial variability of soil nitrate across a long-term agricultural soil, examining the spatial relationships as they change within a 1.2-m depth. These spatial relationships could then be used in the estimation procedure of block kriging, predicting soil nitrate concentrations at unsampled regions within the field.

MATERIALS AND METHODS

A 3.0-ha field, measuring 200-m by 150-m, which had been cropped to continuous winter wheat (*Triticum aesivitum* L.) since 1979, was sampled across a regular grid pattern. The soil at this site was classified as a Pond Creek silt loam (fine-silty, mixed, mesic Pachic Ustoll). A large scale grid covered the entire 3.0-ha, and the soil was sampled at 25-m intervals within this large grid. A smaller .06-ha grid was located at the center of the large grid, and this smaller grid was sampled at 5-m intervals. A total of 99 samples were removed, with 63 and 36 removed from the large and small grids, respectively.

All samples were removed to a depth of 1.2-m, using a Giddings hydraulic soil probe. One soil core (4.5-cm i.d.) was removed at each sampling point and extruded into a plastic sleeve that was sealed and refrigerated until processing. At processing, each core was sectioned into six depths: 0-15, 15-30, 30-45, 45-60, 60-90, and 90-120-cm. All samples were air-dried and ground to pass a 2-mm sieve before further analysis.

Each sample was analyzed for soil NO_3^-, NH_4^+ and pH content. Soil nitrate and ammonium content were determined from 2M KCl extracts (Keeney and Nelson,1982), using colorimetric analysis via a Lachat Flow injection analyzer. Soil pH was determined in a 1:1 soil:H2O solution, using a standard pH electrode. All sample determinations were duplicated, and the duplicate results averaged.

Statistical Analyses

All data were initially analyzed by classical statistical methods, providing estimates of each variable's mean, standard deviation, skew, and coefficient of variation.

Geostatistical analyses were used to describe the spatial variability of soil nitrate content. All classical and geostatistical analyses were performed using the GEOEAS (v 1.1) geostatistical package (Englund and Sparks, 1988). Spatial relationships were described through the use of omnidirectional and directional semivariograms, employing the use of relative semivariograms, as described by Cressie (1985). Relative semivariograms are created when ordinary semivariograms are divided by the square of the mean of the sample values used in the semivariogram calculation. These types of semivariograms are useful when correcting a simple nonstationarity, when the local variance is proportional to the squared local mean (Cressie, 1985). This "proportional effect" is often found in data sets that contain a log-normal distribution (Clark, 1979).

Omnidirectional semivariograms were calculated from every pair of data points within one-half of the total sampled distance, considering every direction at each selected lag distance. Directional semivariograms were calculated over 4 directions: 0, 45, 90, and 135 degrees, each with an angular tolerance of 22.5 degrees. At a given lag distance, all points located within 22.5 degrees of the selected direction were included in the semivariogram calculation, again limited to a final lag length of one-half the total sampled distance. In effect, the four directional semivariograms with an angular tolerance of 22.5 degrees divided the total area described by the omnidirectional semivariogram into four sections.

Directional semivariograms were used to determine if anisotropy existed within the data set. Anisotropies are said to occur if the semivariograms change over varying directions. Semivariograms were calculated over a variety of directions, and the range for a particular semivariance was determined for each semivariogram. These ranges were plotted on a rose diagram, and the major and minor axes of continuity were identified. A rose diagram is a circular or elliptical plot of ranges of directional semivariograms, and the direction and relative size of the ellipse provides information about major and minor axes of continuity within the sampled site.

Models fit to the experimental semivariograms were used in the estimation process of block kriging. Cross-validation was used to check the accuracy of the chosen model(s) intended for the block kriging procedure. Known values at each sampled location were estimated by kriging, and those estimated values were compared to actual. Kriging error, mean of the estimation error and variance of the estimation error was used to determine the accuracy of the chosen model.

Block kriging was used to estimate unknown values across the sampled site. A total of forty-eight 2x2 blocks were estimated throughout the experimental area.

RESULTS AND DISCUSSION

Table 1 (p. 12) lists statistical summaries for soil nitrate values at the six depth increments. There was a wide range in measured soil nitrate at all the depths, indicated by large coefficient of variations (CV) and variances. In an effort to reduce large kriging variances, the two largest outliers from each data set were removed. Although this editing did lessen the presence of extreme outliers, the resulting CVs, variances, and skews shown in Table 1 were still large. This indicated data sets that could be difficult to model and employ in the estimation process of kriging.

The largest measured soil nitrate values were located predominately in the southeast corner of the sampled field, and this region of elevated soil nitrate values was found throughout the entire 1.2-m sampled depth, as shown in Figure 2 (p. 13). There were no obvious drainage patterns or tillage practices that could explain the wide variation in soil nitrate values found within the sampled site. The region of high nitrate did appear to drift slightly southward as soil depth increased, possibly a result of nitrate leaching coupled with the lateral movent of this mobile nutrient.

Constructed semivariograms provided information about the spatial variability of soil nitrate. Omnidirectional semivariograms were fairly well-behaved, usually fitting a spherical model and rising to a well-defined range, as shown in Table 2 (p. 14) and Figure 3 (p. 15). The semivariograms shown and modeled in this figure and table represent general relative semivariograms, or the semivariogram value at each lag divided by the square of the mean of the values used in producing that semivariogram value:

$$\boxed{{}^{*}\gamma(h) = \frac{\gamma(h)}{\text{mean }(h)^2}}$$

(Isaaks and Srivastava, 1989)

It is important to realize that the semivariogram values on the y-axis and the resulting sill and nugget values shown in Figure 3 are *relative* values; they must be multiplied by that lag's mean value in order to achieve actual semivariogram values. This leads to an unfortunate situation: the use of relative semivariograms nicely compensates for a proportional effect, yet produced semivariograms are a function of the squared mean of the values. For example, the apparent low sills found in the semivariograms of the 0-15 and 15-30-cm depth increments are a function of the high squared means that were the divisor at each lag interval. In reality, the sills for both these depths were higher than the remaining soil increments, a reality that is difficult to discern in the relative semivariograms. The benefit of relative semivariograms is apparent in the relatively clean spatial structure found in the semivariograms, allowing precise model fits for the final kriging procedures.

For comparison, traditional semivariograms are shown in Figure 4 (p. 16). These semivariograms demonstrate the higher sill and nugget effects found in the 0-15 and 15-30-cm semivariograms that were hidden by the relative semivariograms. The semivariogram created from the surface soil nitrate values contains the largest nugget and sill, reflecting the larger variability found within this data set. Deeper semivariograms were linear, and it was thought that linear models fit to these semivariograms could be used in the kriging process. However, the cross-validation criteria for these models (not shown) was not as satisfactory as those calculated from the spherical models fit to the relative semivariograms.

Directional semivariograms were created to determine the angles of anisotropy, those directions over which samples were most and least related to each other. As shown in Table 3 (p. 17), the direction in which samples were least related was, at all depths, N135°W. The direction in which soil nitrate was most related changed with depth, moving from directly N at 0-15-cm to a general NW direction deeper in the soil. The direction of greatest relationship found at the soil surface could be developed, in part, from factors such as the direction of tillage and fertilizer-applicator travel. Natural landscape and soil factors such as direction of drainage and impeding layers within the soil would also be a consideration, and it may be that the varying anisotropic axes reflect such a changing soil profile.

The anisotropic ratio is the range of the major axis divided by the range of the minor; an anisotropic ratio of 1.0 signals an isotropic condition, and the spatial variability is the same in all directions. With the exception of the 60-90-cm depth the anisotropic ratio was close to 1.0, as there was not a large difference in the ranges of the directional semivariograms, as shown in Table 2. The larger ranges found in the 90-120-cm depth indicate that soil nitrate is spatially related for a greater distance at that depth. This may be a function of 1) less rooting volume to alter soil nitrate values, 2) limited impact from the surface, such as leached nitrate, and 3) beginning of a relatively continuous parent material.

Spherical models were fit to both the omnidirectional and directional semivariograms. Other model fits, including Gaussian, linear, and nested spherical models, were attempted, but cross-validation indicated that a combination of the omnidirectional semivariograms coupled with the anisotropic angle and major and minor ranges provided a reliable model fit.

Criteria for the cross-validation procedure are found in Table 4 (p. 18). The mean of the estimation errors should be close to zero, and the variance of the errors minimized and equal to the kriging variance. The dimensionless mean square error (DMSE) should equal 1, while the mean normalized error (ME) should be close to zero. There can be other criteria for checking the accuracy of the cross-validation procedure, but these are four commonly used techniques (Samper and Numan, 1989; Unlu, et al.,1990). Although the variance of the estimation errors did equal the kriging variance (P>.05) the variances were not particularly small, a result of the wide variation in measured soil nitrate values.

Figures 4, 5, and 6 indicate the results of the block kriging procedure for three of the soil depths: 0-15, 30-45 and 60-90-cm. Block kriging at all depths was performed at 25-m intervals for a total of 48 estimated blocks across the sampled site. Each figure provides a contour plot of both the estimated soil nitrate values and the kriging standard deviation. Kriging standard deviations help pinpoint those areas that may contain less reliable estimates.

In general, kriged estimates produced reliable maps of estimated soil nitrate contents. In all cases, the kriging standard deviation was smallest at the center of the sampled site, a function of the centered small sampling grid. Kriged estimates in this region would likely come from a larger number of closely spaced samples, which would most likely lower the kriging variance. Likewise, the largest kriging standard deviations were consistently found in the regions of elevated soil nitrate values and those regions where the outliers had been removed. These regions were most likely to contain a large nitrate value in close proximity to a small value, a situation that could create greater error in the estimation process. Kriging standard deviations with the two outliers included in each data set were even larger than those shown in Figures 4, 5, and 6.

It appears that geostatistical methods have applications in exploring the spatial variability of mobile nutrients such as soil nitrate. It does seem, however, that both the data and resultant semivariograms should be viewed with a knowledge of the fields' cultural treatments, particularly in the surface depth. This could be especially true with fertility nutrients--those added to and incorporated into the soil in measurable amounts. Field spatial variability as it is affected by reduced-tillage, erosion control structures such as terraces, or irrigation is another research area that could help explain the spatial variability of soil nitrate and other fertility nutrients.

A geostatistical analysis works well when there are sample numbers adequate to describe the spatial variability of the region of interest. It may be that mobile nutrients such as soil nitrate may require a more intensive sampling scheme than comparable soil physical properties. In this research project, kriging variances were sensitive to regions that were less sampled and highly variable in soil nitrate content. Research will be needed on many sites and soils to determine the minimum number of samples required to accurately describe a region's spatial variability. A spatial description of soil nitrate content within an agricultural field could easily be used in the new computer-aided precision-application fertilizer technologies, eliminating over-fertilization and assisting in the protection of environmental quality.

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Figure 1. Generalized Semivariogram

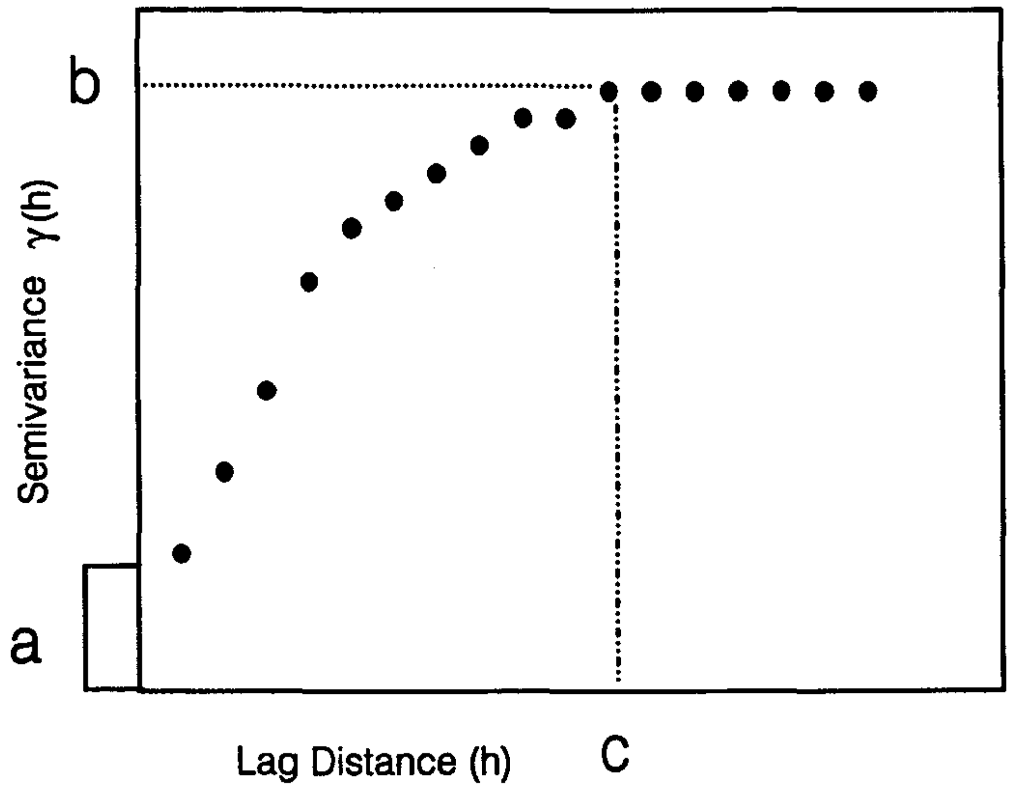


Table 1. Statistical summary for soil nitrate at varying depths

Depth	Mean	Var	Max	Min	CV	skew	kurtosis
---cm---	mg/kg				---%---		
0-15	22.9	39.7	39.3	11.2	27.5	.4	2.4
15-30	8.9	15.0	30.9	3.7	43.3	2.3	12.4
30-45	3.5	8.5	22.1	1.2	84.6	3.9	22.1
45-60	2.8	8.2	15.5	.7	101.6	2.8	10.6
60-90	2.3	5.3	15.4	.5	98.5	3.2	15.4
90-120	2.2	7.3	16.0	.5	125.1	3.4	14.7

Figure 2. Contour Plots of Measured Soil Nitrate Values

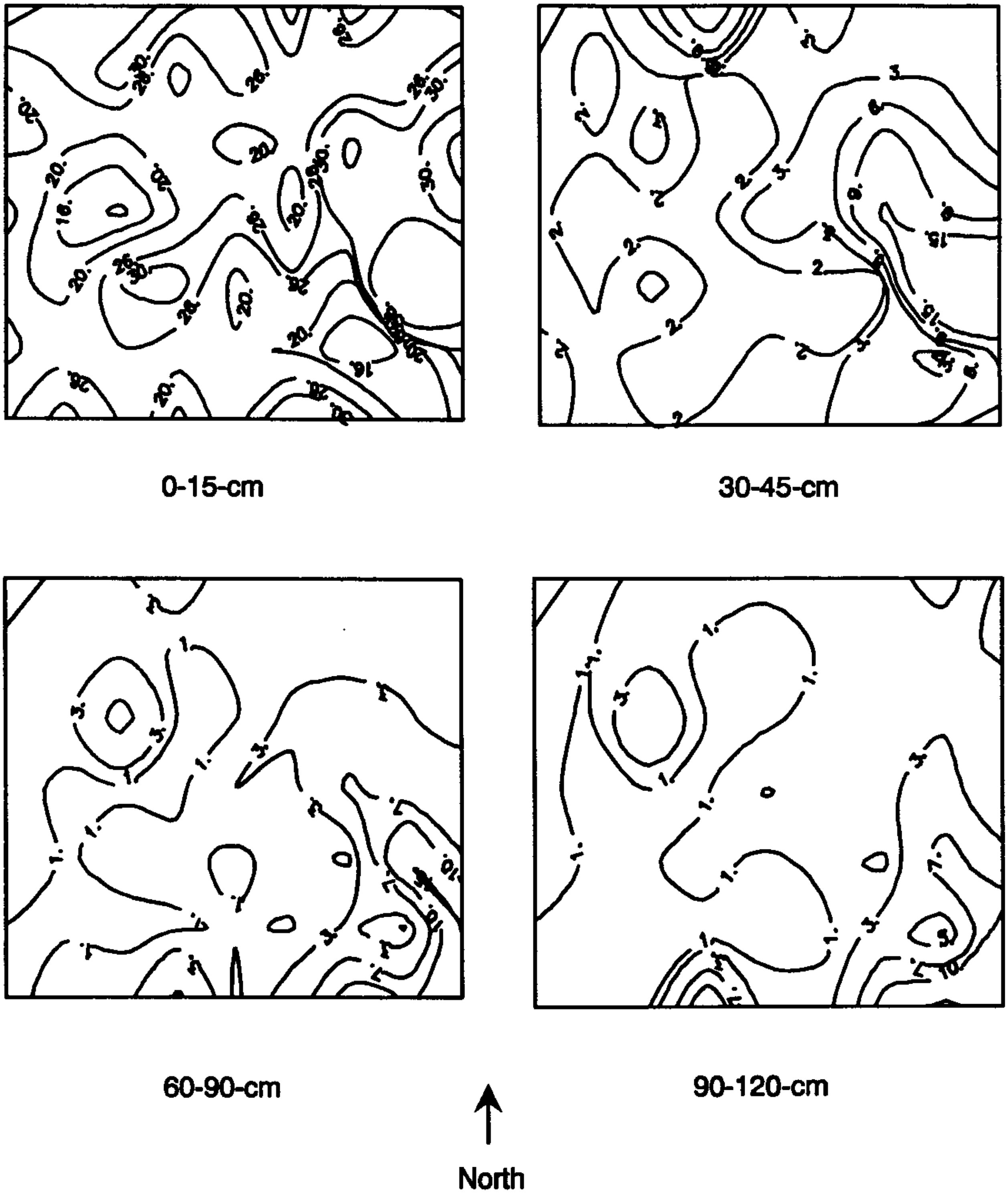


Table 2. Semivariogram parameters relative nugget ,relative sill, range and model type for soil nitrate

Depth ---cm---	Direction	Relative Nugget $(mg/kg)^2$	Relative Sill $(mg/kg)^2$	Range --- m ---	Model
0-15	Omnidirect.	.05	.11	90	Spherical
	N	.09	.02	90	Spherical
	N45°W	.05	.14	90	Spherical
	N90°W	.05	.14	90	Spherical
	N135°W	.07	.05	60	Spherical
15-30	Omnidirect.	.08	.24	90	Spherical
	N	.08	.20	90	Spherical
	N45°W	.05	.35	90	Spherical
	N90°W	.05	.35	90	Spherical
	N135°W	.09	.15	85	Spherical
30-45	Omnidirect.	.05	1.7	95	Spherical
	N	.20	1.2	85	Spherical
	N45°W	.05	1.8	85	Spherical
	N90°W	.05	1.9	95	Spherical
	N135°W	.05	1.2	60	Spherical
45-60	Omnidirect.	.05	1.7	90	Spherical
	N	.20	1.2	90	Spherical
	N45°W	.10	1.9	90	Spherical
	N90°W	.10	2.0	90	Spherical
	N135°W	.10	1.4	70	Spherical
60-90	Omnidirect.	.10	1.1	90	Spherical
	N	.20	.80	95	Spherical
	N45°W	.10	1.2	90	Spherical
	N90°W	.10	1.2	90	Spherical
	N135°W	.15	.65	60	Spherical
90-120	Omnidirect.	.10	1.8	115	Spherical
	N	.10	2.0	115	Spherical
	N45°W	.10	1.9	115	Spherical
	N90°W	.20	1.8	125	Spherical
	N135°W	.20	1.3	95	Spherical

Figure 3. Relative omnidirectional semivariograms for soil nitrate at all soil depths

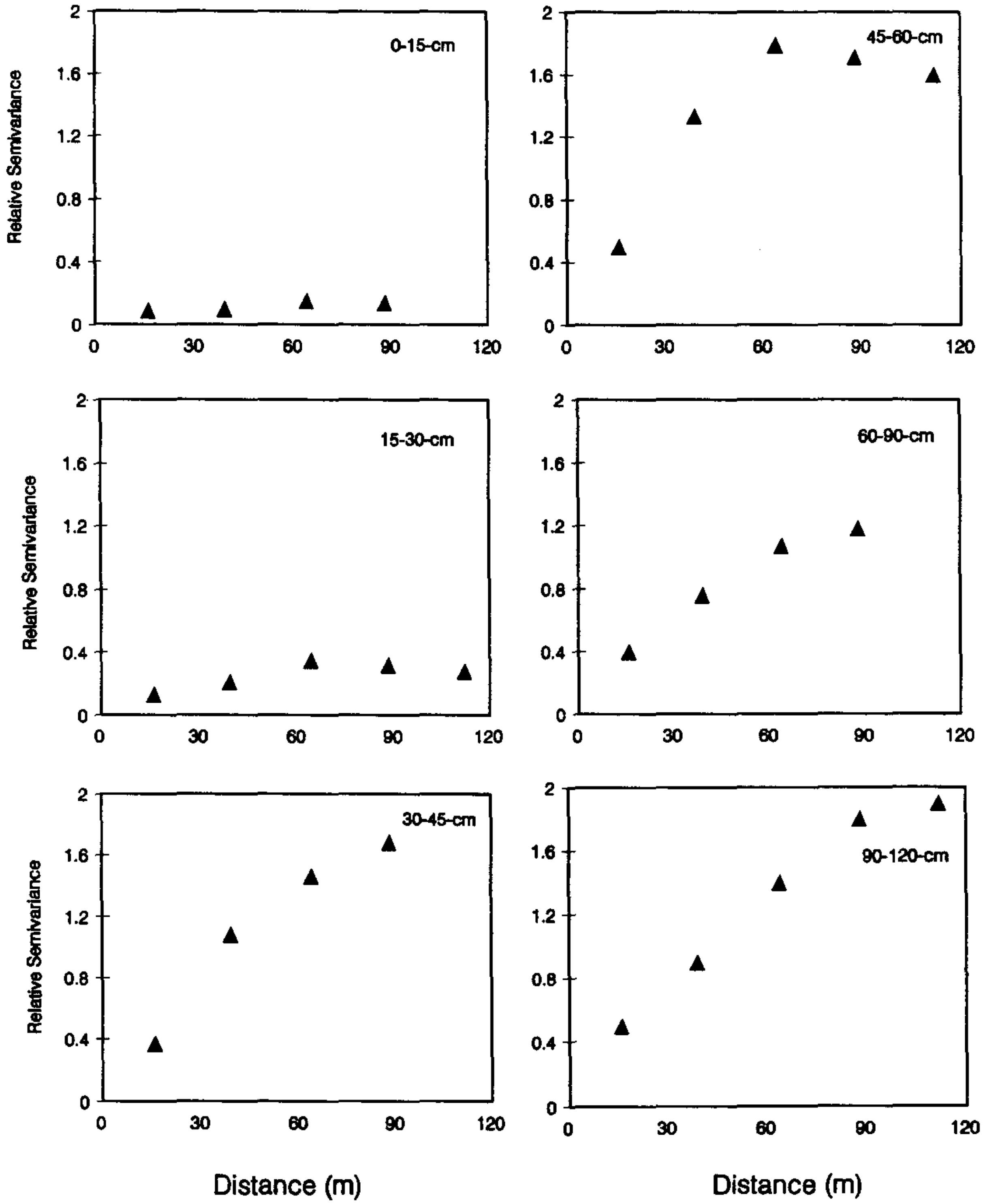


Figure 4. Omnidirectional semivariograms for soil nitrate at all soil depths

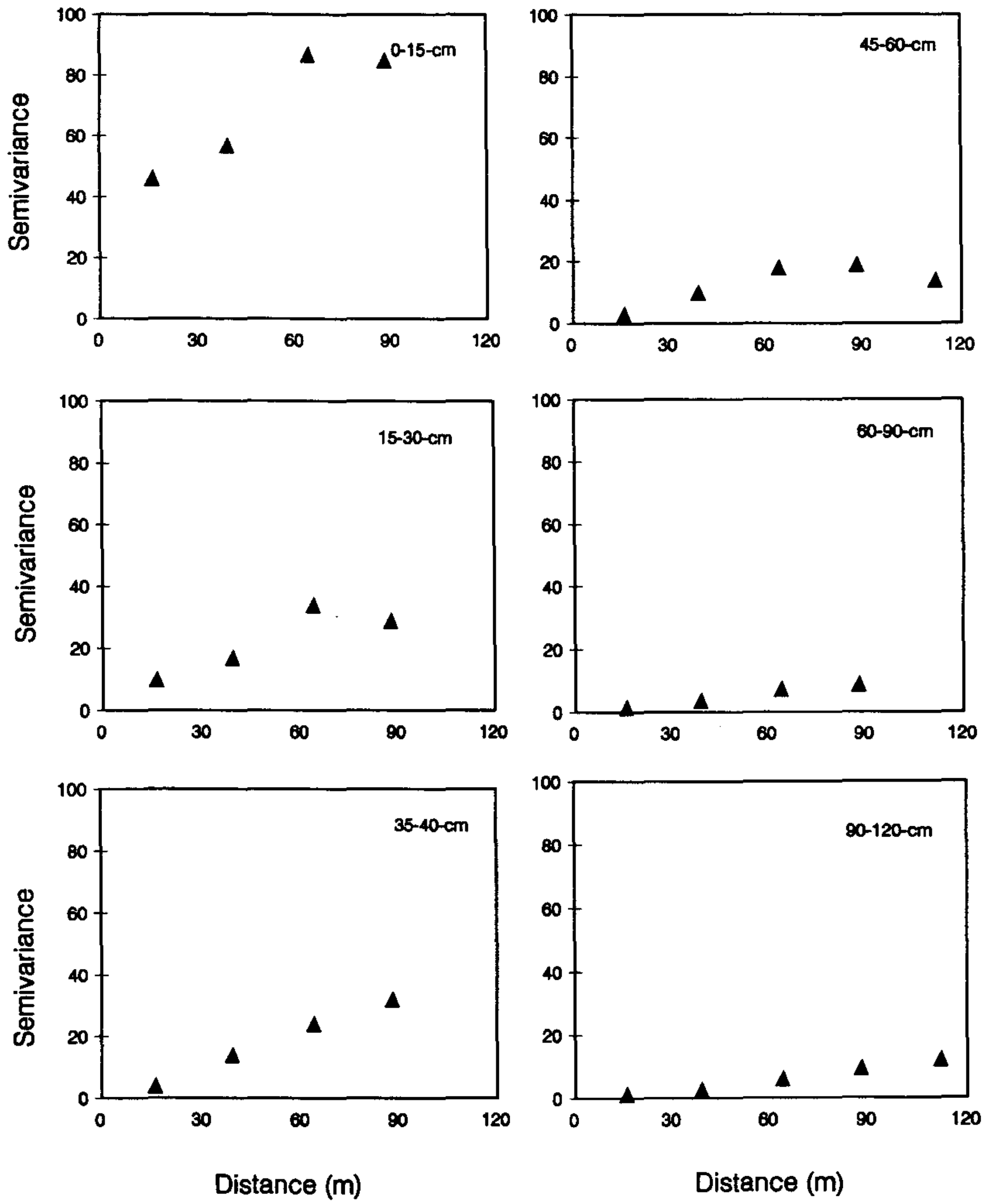


Table 3. Direction of anisotropy as determined by directional semivariograms.

Depth	Major Axis	Minor Axis	Anisotropic Ratio
---cm---			
0-15	N0°W	N135°W	1.5
15-30	N150°W	N135°W	1.1
30-45	N45°W	N135°W	1.5
45-60	N45°W	N135°W	1.3
60-90	N30°W	N135°W	1.9
90-120	N45°W	N135°W	1.2

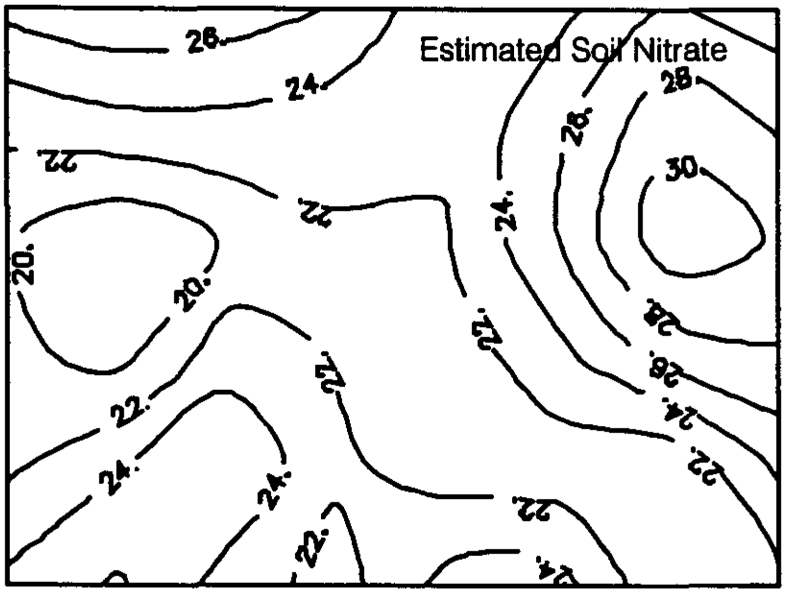
Table 4. Cross-validation criteria for the best-fit models for soil nitrate content at varying depths

Depth ---cm---	Mean Est. Errors	Var. Est. Errors	σ^2_K	DMSE*	ME**
0-15	-.04	42.3	47.1	.94	-.005
15-30	.02	11.6	12.3	.97	.005
30-45	-.02	7.4	6.4	1.1	-.006
45-60	.006	4.0	4.0	1.1	.003
60-90	-.01	2.3	2.2	1.0	-.009
90-120	.001	2.6	2.2	1.1	.001

* Dimensionless Mean Square Error = $\left(\frac{1}{N}\sum \frac{(z_i - z_i^*)^2}{\sigma_K^2}\right)^{1/2}$

** Mean Normalized Error = $\left(\frac{1}{N}\sum \frac{z_i - z_i^*}{\sigma_K}\right)$

Figure 5. Kriged Values and Kriging Standard Deviations for Soil Nitrate 0-15-cm Soil Depth



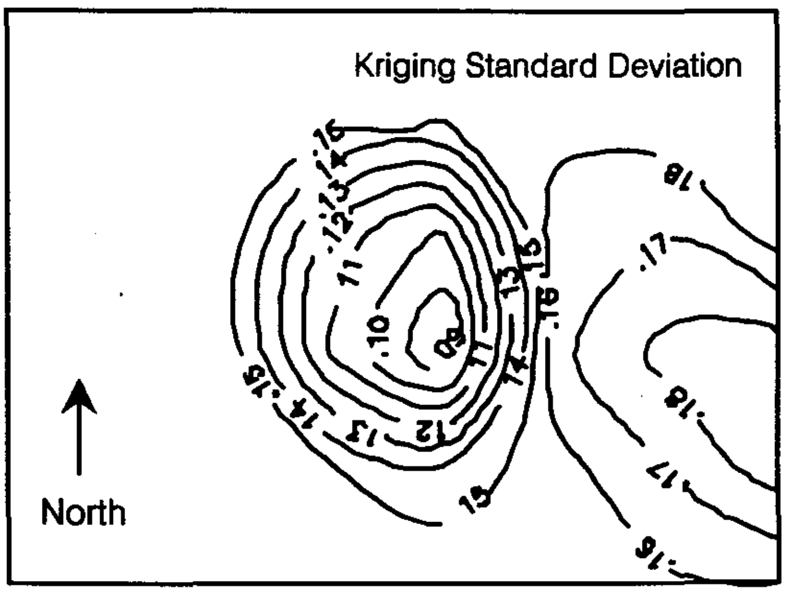


Figure 6. Kriged Values and Kriging Standard Deviations for Soil Nitrate
30-45-cm

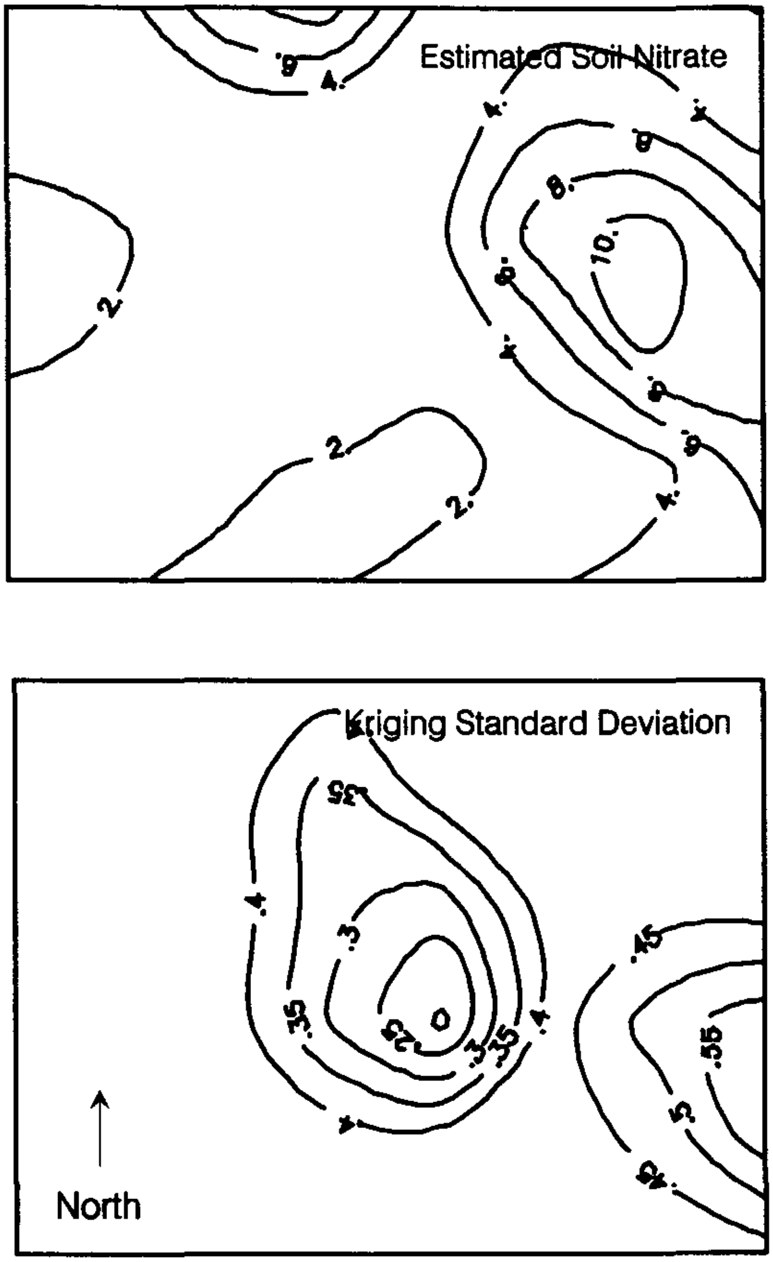
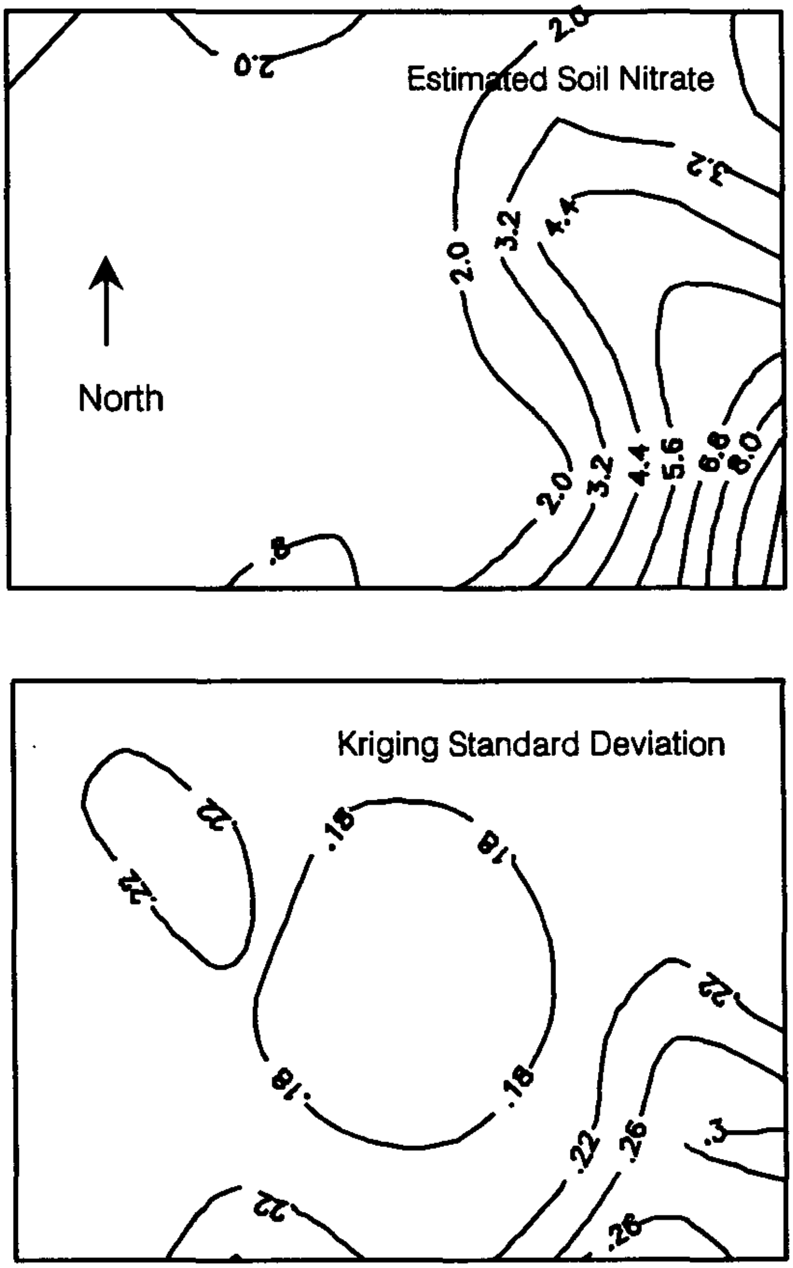


Figure 7. Kriged Values and Kriging Standard Deviations
for Soil Nitrate
60-90-cm



GEOSTATISTICAL ASSESSMENT OF THE SPATIAL VARIABILITY OF SOIL NITRATE IN AN AGRICULTURAL FIELD

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