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ORIGINAL ARTICLE

Spatial analysis of land use and shallow groundwater vulnerability in the watershed adjacent to Assateague Island National Seashore, Maryland and Virginia, USA

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Abstract Spatial relations between land use and groundwater quality in the watershed adjacent to Assateague Island National Seashore, Maryland and Virginia, USA were analyzed by the use of two spatial models. One model used a logit analysis and the other was based on geostatistics. The models were developed and compared on the basis of existing concentrations of nitrate as nitrogen in samples from 529 domestic wells. The models were applied to produce spatial probability maps that show areas in the watershed where concentrations of nitrate in groundwater are likely to exceed a predetermined management threshold value. Maps of the watershed generated by logistic regression and probability kriging analysis showing where the probability of nitrate concentrations would exceed 3 mg/L (>0.50) compared favorably. Logistic regression was less dependent on the spatial distribution of sampled wells, and identified an additional high probability area within the watershed that was missed by probability kriging. The spatial probability maps could be used to determine the natural or anthropogenic factors that best explain the occurrence and distribution of elevated concentrations of nitrate (or other constituents) in shallow groundwater. This information can be used by local land-use planners, ecologists, and managers to protect water supplies and identify land-use planning solutions and monitoring programs in vulnerable areas.

Keywords Groundwater · Geostatistics · Spatial statistics · Logistic regression · Probability kriging

Introduction

Assateague Island National Seashore (AINS) was established by Congress on September 21, 1965 to preserve and protect the natural resources and recreational value of Assateague Island, Maryland and Virginia, USA. AINS is an important natural resource visited by more than two million people annually, showcasing one of the few remaining undeveloped barrier-island environments along the Mid-Atlantic Coast (Fig. 1).

The extensive aquatic and wetland resources of Assateague Island and the adjacent inland coastal bays of Delaware, Maryland, and Virginia, encompass approximately 1,179 km^2 and are central to the significance of AINS. These waters and associated biota are a key part of the recreational use of AINS, as more than 65% of the visits to AINS involve the direct use of aquatic habitats. Chincoteague, Sinepuxent and Newport Bays lie landward of the Assateague barrier island (Fig. 1), while the Isle of Wight and Assawoman Bays to the north are part of the extensive network of coastal bays along the Delaware, Maryland, and Virginia coast. Combined, these five bays comprise an approximately 756 km^2 watershed and extend nearly 80 km from north to south, with an east to west average of about 17 km. The bays are shallow, with an

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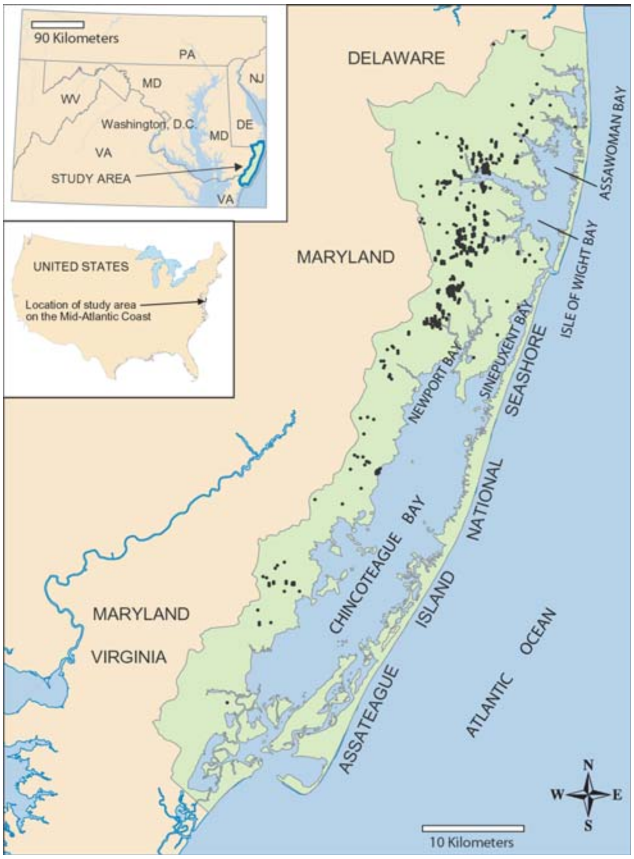

Fig. 1 Assateague Island National Seashore, adjacent watershed and groundwater sampling locations in the shallow aquifer

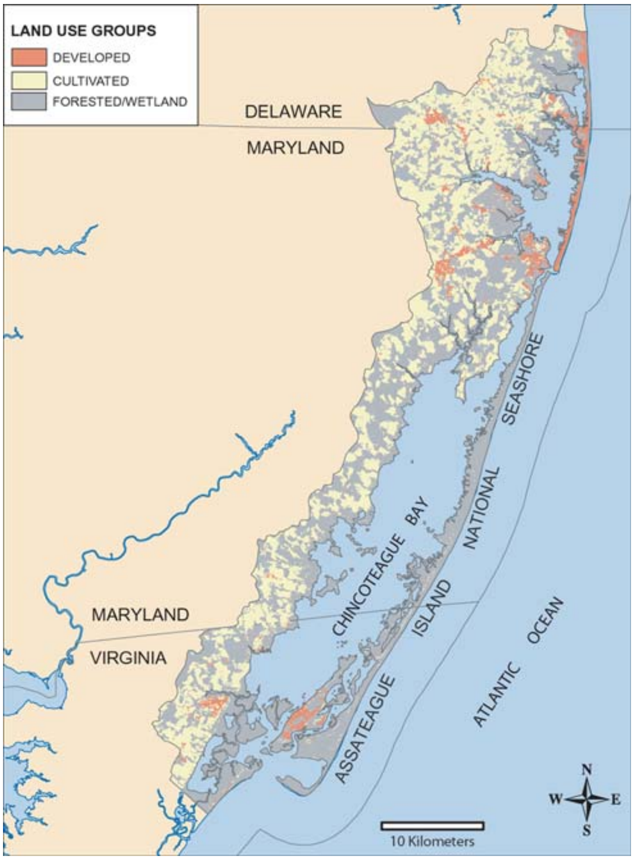

Fig. 2 Distribution of land use in the watershed adjacent to Assateague Island National Seashore

average depth of less than 2 m, and are poorly flushed because of limited freshwater inflow and a restricted tidal exchange through the two inlets, which produces a tidal range of less than a third of a meter (National Oceanic Atmospheric Administration 1990; Maryland Department of the Environment 1993). Due to their physical and hydrologic characteristics, the coastal bays are inherently at risk from pollution and are experiencing significant anthropogenic stress.

Stresses on the coastal bays ecosystem

The marine and estuarine resources of AINS are increasingly threatened by a variety of activities within and outside park boundaries. Environmental degradation is generally related to the distributions of land use within the watershed, development, and population density, and flushing rates for bay water (Fig. 2). The primary threats to the estuarine resources from the upland watershed are agricultural activities, residential and commercial development, consumptive uses such as commercial and recreational fishing, and alteration of the natural coastal processes.

Known stressors include excessive nutrient inputs from point and nonpoint sources, increased turbidity from suspended sediment and phytoplankton blooms, contamination of sediments by nonpoint toxic pollutants, and changes in freshwater inflow. Of these, excessive nutrients are considered to be the most significant long-term threat to the health of the ecosystem (Maryland Department of the Environment 1993).

The relation between groundwater quality on the watershed and the transport of nutrients to the coastal bays is not well defined. Dillow and Greene (1999) determined that the nitrate as nitrogen in groundwater discharge accounts for a significant part of the total load of nitrogen to the Maryland coastal bays environment. On the basis of a simple water-budget approach and limited data, they estimated the potential load of nitrogen to the Maryland coastal bays from direct discharge of nitrates in groundwater to be approximately 123,400 kg/year (approximately 24% of direct discharge). Further investigations on groundwater quality and discharge to the bays showed that dissolved nitrates are the dominant nutrients in groundwater, with concentrations ranging from about 0.05 to 15.5 mg/L (Dillow et al. 2002).

Spatial statistical models

Spatial statistical models provide data analysis and inference techniques that can be used to draw conclusions from geographically referenced and indexed data. Models may range from visualization and exploration of spatial data to sophisticated spatial statistics (geostatistics, state-space, autoregression). In particular, spatial statistics provide a body of methods for spatial smoothing and use techniques that are intended to explore and demonstrate the presence of dependence between observations in space.

Spatial assessments of groundwater quality are complicated by the fact that constituent concentrations are commonly highly variable. Therefore, to characterize the spatial quality of groundwater in an area, the assessment must use a large number of samples from wells that are distributed throughout the study area. In addition, factors that influence groundwater quality must be understood so that management practices or sampling can be targeted to areas that are most vulnerable to contamination.

The US Environmental Protection Agency (USEPA) (1996a) has suggested that nitrate concentrations can be used as indicators of overall groundwater quality. Therefore, nitrate was selected for evaluation in this investigation because elevated concentrations of this constituent are typically caused by anthropogenic activities (crop fertilizer, domestic on-site sewage disposal). In addition, nitrates are more frequently sampled than other constituents. Spalding and Exner (1993) hypothesized that nitrates may be the most widespread contaminant in groundwater. Due to the extensive presence of this contaminant, nitrate concentrations in groundwater may help identify environments that are susceptible to contamination (USEPA 1996a).

Although the most obvious negative implications of contaminated groundwater from nitrates are the direct effects to human health through drinking water, there are wider ecological issues that need to be considered. When groundwater flow contributes significantly to river base flows, for example, there may be associated risk with nitrate contamination above a threshold level that could degrade the environment. Although there is much discussion in the literature about what this threshold level should be, it is generally accepted that concentrations above some ‘‘background’’ level may be used. Nitrate concentrations in groundwater greater than 2–3 mg/L are likely caused by anthropogenic sources and are therefore considered to be a conservative concentrations (Tesoriero and Voss 1997; Muller and Helsel 1996).

This paper explores two types of statistical models—logistic-regression, or logit, and geostatistics—that can be used to determine the natural or anthropogenic factors that best explain the occurrence and distribution of elevated concentrations of nitrate in shallow groundwater. A predictive spatial statistical relation between land use and groundwater was developed and a groundwater vulnerability assessment of the watershed adjacent to AINS was mapped to identify areas that are most susceptible to contamination.

Descriptive statistics of nitrate data

During 2003, water-quality data on nitrate concentrations in 529 wells completed in the shallow unconfined aquifer (less than 30 m) were compiled for this study from existing County Health Department records (Delaware, Maryland, and Virginia) and from US Geological Survey (USGS) data stored in the GWSI (groundwater well-site files) and QWDATA (water-quality) databases. These databases contain well-location, construction, and water-quality parameter information. The locations of groundwater sampling sites are shown in Fig. 1.

Summary statistics of the nitrate data for the 529 wells sampled are shown in Table 1. The mean of the nitrate concentration data in shallow groundwater is 1.43 mg/L. The range of nitrate concentrations in this dataset (combined small domestic, large water supply,

Table 1 Summary statistics of nitrate concentrations as nitrogen in the shallow aquifer (<30 m) in the watershed adjacent to Assateague Island National Seashore

Statistic	Value	Natural log
Number of samples	529	529
Minimum	0.11	–2.21
Maximum	19.70	2.68
25th Percentile	0.37	–1.01
Median	0.88	–0.13
75th Percentile	1.63	0.48
Mean	1.43	–0.21
Variance	3.57	1.12
Standard deviation	1.89	1.06
Coefficients of variation	132.73	500.11
Skewness	3.912	0.04
Kurtosis	26.69	2.48

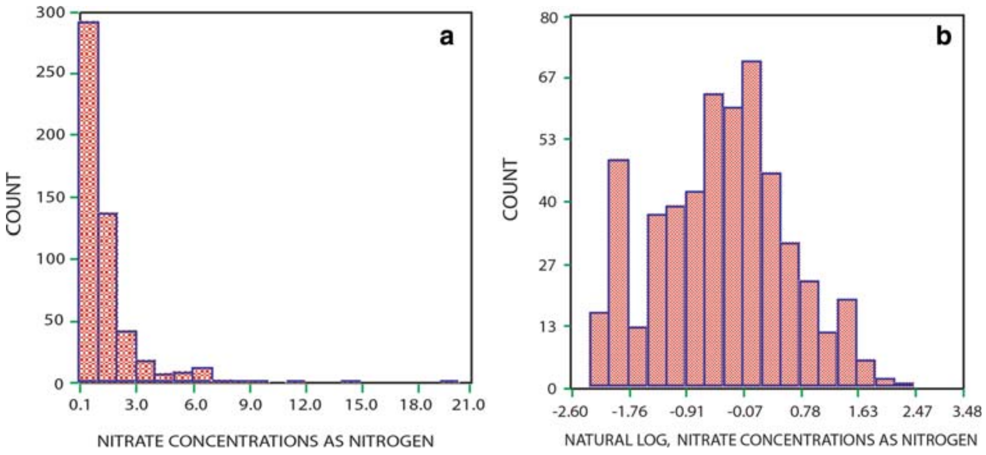

Fig. 3 Distribution of nitrate concentrations as nitrogen from wells sampled in the shallow aquifer (<30 m) of the watershed adjacent to Assateague Island National Seashore: **a** sampled values and **b** natural log transformation

and USGS observation wells) ranged from 0.11 to 19.7 mg/L. This is similar to the range (0.05–15.5 mg/L) reported by Dillow et al. (2002), who only sampled a limited number of USGS observation wells. The histogram plot (Fig. 3) and the statistical summary (Table 1) show that the skewness (3.912) reveals asymmetry on the right side and the kurtosis (26.69) shows a stretching of the distribution of the data. The log-normal transformation of the nitrate concentration data normalizes the data and reduces this asymmetry. Further analysis of the nitrate concentration data showed 4 of 529 wells (<1%) had nitrate concentrations above the USEPA maximum contaminant level (MCL) of 10 mg/L for nitrates (USEPA 1996b). Assuming a background level (environmental threshold) of 3 mg/L, 58 of 529 wells (about 11%) showed likely anthropogenic nitrate contamination in groundwater.

Logit analysis of nitrate data

Land use and geologic type have previously been related to the occurrence of elevated nitrate concentrations in groundwater throughout the Mid-Atlantic Region (Ator and Ferrari 1997; Nolan 2001). Greene et al. (2005) developed a regional spatial statistical model (logit) that utilized these variables with other geographic data to predict the vulnerability of groundwater to elevated concentrations of nitrates in the Mid-Atlantic. Groundwater vulnerability of groundwater to nitrate contamination was modeled using water-quality data from 927 sites throughout the region. Spatial probability maps showing the likelihood of elevated concentrations of nitrates in groundwater being above a certain threshold or indicator value for the region along with their associated uncertainty were developed and displayed (Greene et al. 2005).

The methodology used to predict the vulnerability of groundwater to nitrate contamination (Greene et al. 2005) was applied to the watershed adjacent to AINS. The logit statistical model was developed by relating statistically significant geographic variables to the 529 nitrate samples from the watershed and predicting the likelihood that nitrates in the shallow groundwater would occur above a threshold of 3 mg/L.

The response probability, p_i, of the logit model (Eq. 1) can be defined as

$$p_i = P(Y = 1|X_i) = \frac{e^{(\beta_0+\beta_1 x_{i1}+\beta_2 x_{i2}+\cdots+\beta_k x_{ik})}}{1 + e^{(\beta_0+\beta_1 x_{i1}+\beta_2 x_{i2}+\cdots+\beta_k x_{ik})}}, \qquad (1)$$

where for each of the n observations there is a response Y_i, which can take on the values of 1 or 0, from corresponding independent explanatory variables X_i, $i = 1, 2, \ldots, n$, where $X_i = (1, X_{i1}, X_{i2}, \ldots, X_{ik})$ and k represents the regression coefficient corresponding to the kth explanatory variable, with β_0 representing the intercept. The vector $\beta = (\beta_0, \beta_1, \beta_2, \ldots, \beta_k)$, is called the vector of slope parameters. Equation 1 can be simplified further by dividing both the numerator and denominator by the numerator itself to get a form of the logit equation (2) that has a desired property of no matter what is substituted for X_i, and β_i, the probability p_i, will always be between 0 and 1.

$$p_i = P(Y = 1|X_i) = \frac{1}{1 + e^{(-\beta_0-\beta_1 x_{i1}-\beta_2 x_{i2}-\cdots-\beta_k x_{ik})}}. \qquad (2)$$

Several authors have shown that there is a significant relation between shallow groundwater quality (nitrate concentrations) and land use near a sampled well (Cain et al. 1989; Hay and Battaglin 1990; Barringer et al. 1990; Tesoriero and Voss 1997; Greene et al. 2005). In developing the logit model for nitrates in the watershed, land use within an optimal radius was used to establish an area of influence around each well (Fig. 4). The optimal land-use radius was determined by analyzing how well the logit models at different radii fit the nitrate data. Logit models for 30 radii that ranged from 100 to 3,100 m in 100-m increments were tested. The best-fit model was determined by finding the radii that maximized the likelihood ratio test (G statistic) (Hosmer and Lemeshow 1989). The best-fit model that maximized the G statistic for nitrate concentrations exceeding a threshold of 3 mg/L was determined to be 1,300 m (Fig. 4).

The logit model for the AINS watershed was developed by individually testing selected variables to determine if they were significant predictors ($p < 0.05$) of elevated nitrate concentrations above a 3 mg/L threshold. Logit models that were considered and tested included land use, surficial geology, soil permeability, soil organic matter, depth of soil layer, depth to water table, soil texture, hydrologic soil groups, manure, fertilizer, atmospheric deposition, and population density. Significant single variable logit models were combined into a multivariate logit model that used significant explanatory variables to predict the probability of nitrate concentrations exceeding a threshold of 3 mg/L.

The logit model was developed using goodness-of-fit statistical procedures [likelihood ratio test (G) and Hosmer and Lemeshow (H–L test) statistics] to define the final logit model (Hosmer and Lemeshow 1989). Regression coefficients and statistics for explanatory variables that were significant predictors are presented in Table 2.

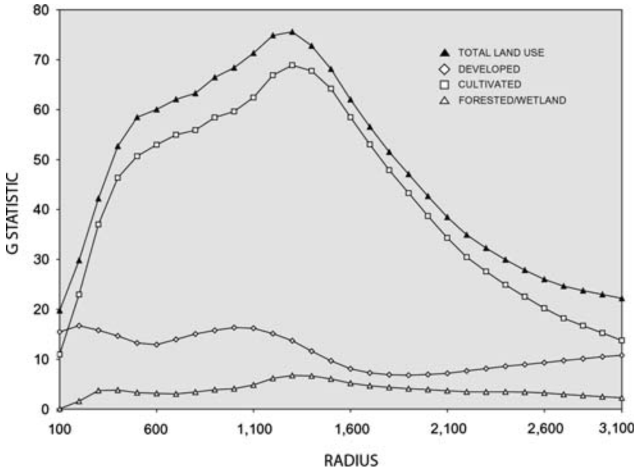

Fig. 4 Land-use radius analysis for best-fit (G statistic) logistic regression model for nitrate concentration as nitrogen in groundwater exceeding a 3 mg/L threshold in the watershed adjacent to Assateague Island National Seashore

Table 2 Beta (β) coefficients and corresponding *p*-values for the logit model used to estimate the probability that nitrate concentrations as nitrogen in groundwater will exceed the 3 mg/L threshold

Variable	Beta (β) coefficient	Values	*p* Values
Intercept	β_0	–7.98	<0.0001
Cultivated land use	β_1	0.09	<0.0001
Hydrologic soils group C	β_2	0.14	0.0099
Population density	β_3	0.02	0.0010

After developing the best-fit logit model to determine the probability of nitrate in groundwater exceeding a threshold of 3 mg/L, a geographic information system (GIS) was used to generate an array of regularly spaced points on a 1,300-m grid representing the watershed. These points represent the center of each grid cell and correspond to the center of the 1,300 m radius that was determined to be the best-fit model from the land-use analysis (Fig. 4). Logit model coefficients (Table 2) that were developed from the explanatory variables (Eq. 2) were applied to each point on the grid and maps that displayed the probability of nitrate concentrations exceeding a threshold of 3 mg/L were developed. These maps show the vulnerability of groundwater to nonpoint nitrate contamination exceeding this threshold level (Fig. 5a).

In addition to the probability estimates, the uncertainty of the probability estimates in the form of confidence maps was generated and displayed. The length of the confidence interval helps discern the error in the probability estimate. The upper bound of the confidence interval for each estimate can be thought of as the worst-case scenario, or highest possible probability, of nitrate concentrations in groundwater exceeding a 3 mg/L threshold within a 95% confidence interval (Fig. 5b).

Geostatistical analysis of nitrate data

Geostatistics is the analysis of data that are distributed in space and (or) time (Olea 1991). This analysis can account for location and (or) time of measurement, which is crucial to understanding the spatial patterns and interpolating the value of the attribute of interest at unsampled locations. Therefore, geostatistical analysis offers a set of tools and methods aimed at understanding and modeling the spatial variability of the data (de Marsily 1986; Dagan 1989; Goovaerts 1997; Deutsch and Journal 1998).

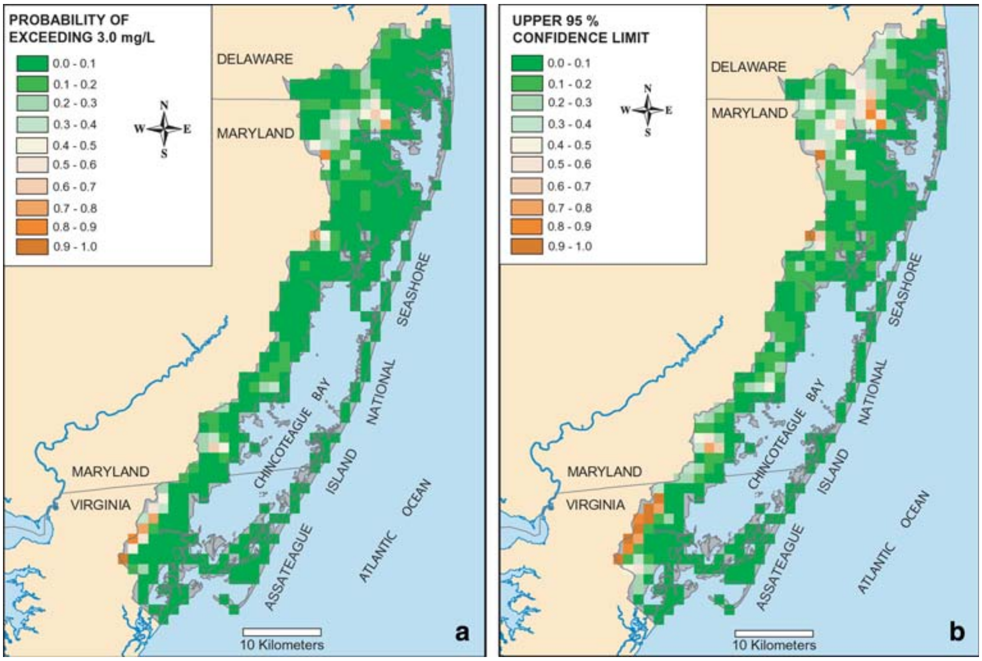

Fig. 5 Logistic regression model of: **a** probability of nitrate concentrations as nitrogen in groundwater exceeding a 3 mg/L threshold, and **b** upper limit of the 95% confidence interval in the shallow aquifer of the watershed adjacent to Assateague Island National Seashore

Kriging (geostatistical prediction) refers to a set of "generalized linear regression techniques for minimizing the estimation variance defined from a prior model for covariance" (Olea 1991). Several types of kriging methods can be used to quantify the spatial structure of the data and produce predictions. The method chosen depends on the assumptions made about the data structure and the model. Most kriging methods are based on the assumption that the attribute to be predicted has a continuous range of possible outcomes and can be modeled by using a continuous random variable (RV) (Goovaerts 1997). The basic ordinary kriging model is

$$Z(s) = \mu(s) + e(s), \tag{3}$$

where $Z(s)$ is the variable of interest at some location $[s = (X, Y)]$, which is decomposed into a trend $\mu(s)$ with random, autocorrelated errors $e(s)$. The simplest ordinary kriging model attempts to predict the unknown values based on location; a constant mean, m, for the data (no trend); and accounts for random errors with spatial dependence. On the basis of the nitrate dataset for the watershed adjacent to AINS, the best-fit directional semivariogram is shown in Fig. 6a. The directional influences of the nitrate data were significant and were incorporated into the variogram analysis. This directional influence was strongest at an angle of 24° east of north (Fig. 6a, b), which indicates that nitrate concentrations in groundwater in the watershed adjacent to AINS were more similar between sampled wells in this direction than in any other. The preferential direction of 24° east of north may be due to the distribution of sampled wells, or the prevailing direction of shallow groundwater flow.

The kriging model described in this paper is a variation of the basic Eq. 3 and uses an indicator RV (discrete RV) with two possible outcomes: 0 and 1. These binary outcomes are analogous to the outcomes that were used in the logit model. The model is known as a "probability kriging model". This type of kriging produces a spatial distribution of the probability of exceeding a threshold or standard errors of indicators and can be compared to the probability of exceeding a threshold distribution that is developed by use of the logit model. The probability kriging model is

$$I(s) = I(Z(s) > c_t) = \mu_1 + e_1(s), \tag{4}$$

$$Z(s) = \mu_2 + e_2(s), \tag{5}$$

and

$$I(s) = \begin{cases} 1 & \text{if } Z(s) \geq c_t, \\ 0 & \text{if } Z(s) < c_t, \end{cases} \tag{6}$$

where μ_1 and μ_2 are unknown constants and $I(s)$ is the binary variable determined by whether the variable of

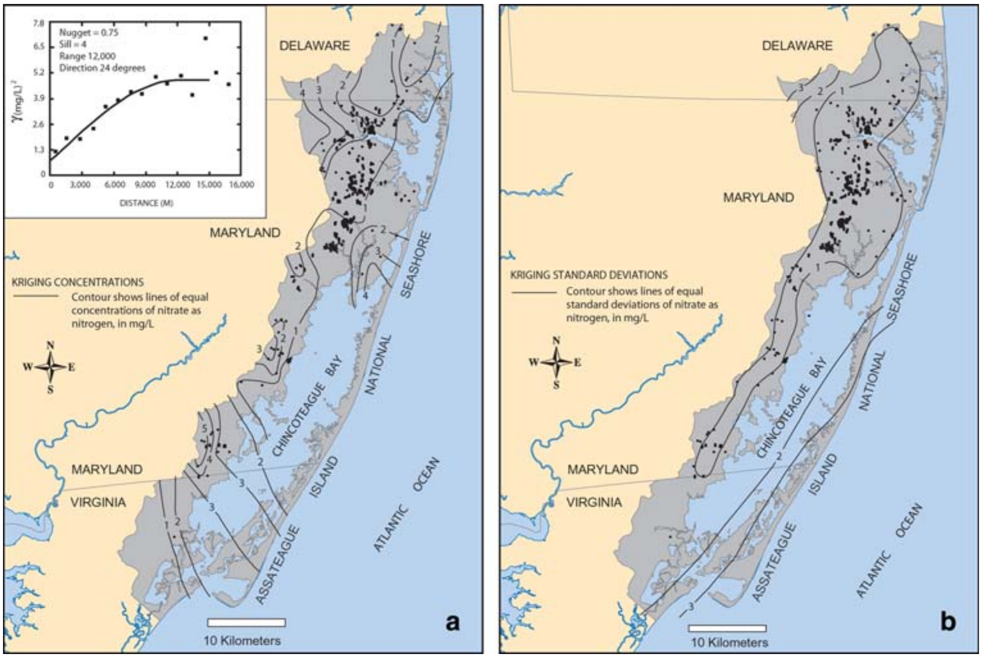

Fig. 6 Ordinary kriging of the spatial distribution of nitrate concentrations as nitrogen for the watershed adjacent to Assateague Island National Seashore: **a** best-fit directional semivariogram model and kriging results, in mg/L, and **b** standard deviations, in mg/L

interest $Z(s)$ is greater or less than the threshold c_t. One major difference and complication of using probability kriging over ordinary kriging is that there are two error terms, $e_1(s)$ and $e_2(s)$. Thus, there is an autocorrelation associated with each e_i and a cross-correlation between them that must be evaluated. Probability kriging can be used to evaluate the probability at any location that the variable of interest Z (nitrate concentrations in groundwater) will exceed the threshold c_t (3 mg/L).

The spatial autocorrelation of the nitrate concentration data from groundwater samples in the watershed adjacent to AINS was explored by modeling with semivariograms. The best-fit experimental semivariogram with the incorporation of the directional influences is shown in Fig. 6a.

By crossing the variable of interest (nitrate concentrations in groundwater) with land use, the cross-correlation can be evaluated and analyzed. The experimental cross-variogram between nitrate concentrations and land use (Fig. 7) shows a strong spherical model correlation, and a significant spatial correlation between nitrate concentrations in groundwater and land use. A cross-validation analysis was conducted on the best-fit semivariogram model to determine how well the model predicts the unknown values. The statistical prediction error is the difference between the predicted and actual measured values. Models can be evaluated by using two common diagnostic statistics, the mean error and the root-mean-square-standardized error. For a model that provides accurate predictions, the mean error should be close to 0 and the root-mean-square-standardized error should be close to 1. For this model, the mean error is 0.003 and the root-mean-square-standardized error is 0.962.

The probability of nitrate concentrations exceeding a 3 mg/L threshold based on an indicator kriging model is presented in Fig. 8a. In addition, an error map of the estimation variances for the probability that nitrate concentrations in groundwater will exceed 3 mg/L is shown in Fig. 8b.

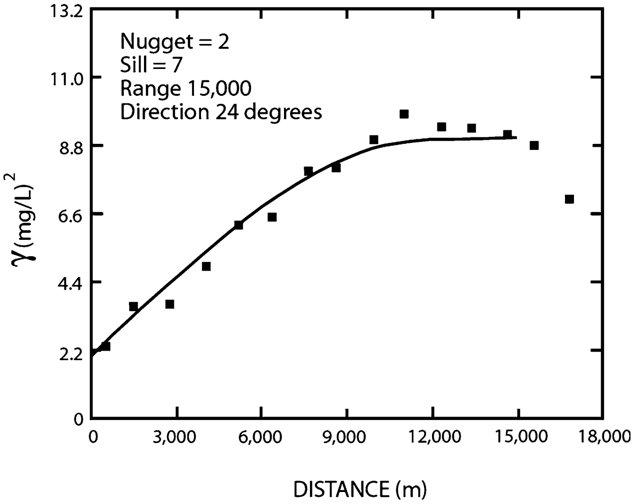

Fig. 7 Cross-variogram model of nitrate concentrations as nitrogen and cultivated land use in the shallow aquifer of the watershed adjacent to Assateague Island National Seashore

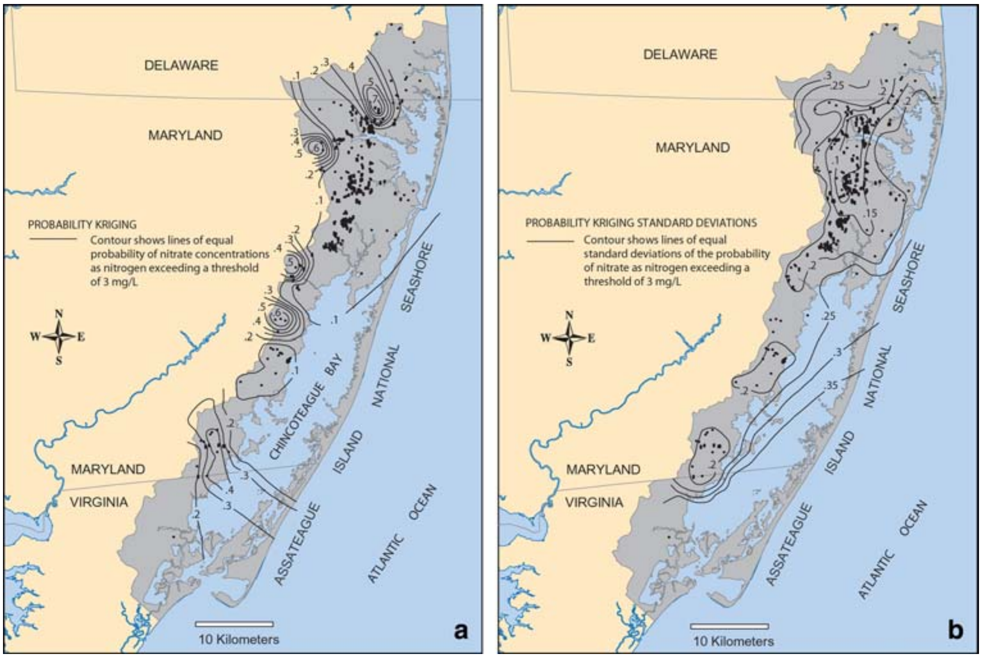

Fig. 8 Probability kriging of nitrate concentrations as nitrogen in the shallow aquifer of the watershed adjacent to Assateague Island National Seashore: **a** probability of exceeding a threshold of 3 mg/L, and **b** standard deviations

Results and discussion

A logit (logistic-regression) model was developed to characterize and predict the spatial probability that nitrate concentrations as nitrogen in groundwater will exceed a 3 mg/L threshold. The logit model used a dependent variable (nitrate concentrations in groundwater) and three significant explanatory variables (cultivated land use, hydrologic soils group C, and population density) to quantify the relation between geographic factors and the probability that nitrate concentrations in groundwater will exceed a specified concentration threshold of 3 mg/L. Throughout much of the shallow groundwater in the watershed adjacent to AINS, there is a low probability (<0.5) that nitrates will exceed 3 mg/L. In several areas however, there is a high probability (>0.5) of exceeding the threshold, which in some cases approaches 1 (>0.9). The areas with the highest probabilities are in the southwestern part of the Chincoteague Bay watershed draining from Virginia, and the watershed area draining into Assawoman Bay. Throughout most of the central part of the Chincoteague Bay watershed, the probability of nitrate exceeding 3 mg/L was less than 50% (<0.5), except in isolated areas where probabilities were equal to or greater than 0.5 (Fig. 5).

The results of the geostatistical (probability kriging) approach used to predict whether nitrate concentrations would exceed 3 mg/L closely matched the results from the logit model in the Assawoman Bay watershed and isolated areas in the central part of the Chincoteague Bay watershed. The predicted probabilities between the two models differed in the Virginia part of the watershed adjacent to AINS, where probability kriging did not show a high probability of nitrate concentration exceeding 3 mg/L. This was likely due, however, to the lack of groundwater quality data in that area needed for the probability kriging estimates.

Probability kriging is dependent on the spatial distribution and coverage of sampled wells. If an area is missing data (or contains no sampled wells), then geostatistics cannot be used to make probability estimates because there is no spatial autocorrelation between wells. In these cases either estimates cannot be made or the standard deviation is large (Fig. 8b); however, the logit model uses the existing data (nitrate from sampled wells) to develop the spatial relation between the dependent variable and mapped geospatial explanatory variables.

These types of analyses that use existing data could assist managers and help determine the natural or anthropogenic factors that best explain the occurrence and distribution of elevated concentrations of nitrate (or other constituent) in shallow groundwater. Spatial statistics can be used by local land-use planners, ecologists, and managers to protect water supplies and identify effective land-use planning solutions and monitoring programs in vulnerable areas.

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