Estimation of regionalized phenomena by geostatistical methods: lake acidity on the Canadian Shield

C. Bellehumeur · D. Marcotte · P. Legendre

Abstract This paper describes a geostatistical technique based on conditional simulations to assess confidence intervals of local estimates of lake pH values on the Canadian Shield. This geostatistical approach has been developed to deal with the estimation of phenomena with a spatial autocorrelation structure among observations. It uses the autocorrelation structure to derive minimum-variance unbiased estimates for points that have not been measured, or to estimate average values for new surfaces. A survey for lake water chemistry has been conducted by the *Ministère de l'Environnement du Québec* between 1986 and 1990, to assess surface water quality and delineate the areas affected by acid precipitation on the southern Canadian Shield in Québec. The spatial structure of lake pH was modeled using two nested spherical variogram models, with ranges of 20 km and 250 km, accounting respectively for 20% and 55% of the spatial variation, plus a random component accounting for 25%. The pH data have been used to construct a number of geostatistical simulations that produce plausible realizations of a given random function model, while 'honoring' the experimental values (i.e., the real data points are among the simulated data), and that correspond to the same underlying variogram model. Post-processing of a large number of these simulations, that are equally likely to occur, enables the estimation of mean pH values, the proportion of affected lakes (lakes with $pH \leq 5.5$), and the potential error of these parameters within small regions (100 km × 100 km). The method provides a procedure to establish whether acid rain control programs will succeed in reducing acidity in surface waters, allowing one to consider small areas with particular physiographic features rather than large drainage basins with several sources of heterogeneity. This judgment on the reduction of surface water acidity will be possible only if the amount of uncertainty in the estimation of mean pH is properly quantified.

Key words Acid rain · Conditional simulations · Confidence intervals · Geostatistics · Lake acidity

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Introduction

Several environmental and ecotoxicological problems require the estimation of the average value of a variable calculated within a certain area. The estimation of the mean value of the concentration of a pollutant allows one to evaluate potential ecological and health hazards, and to make environmental decisions (such as soil remediation, design of new regulation, etc.). Because an estimate is based upon a fraction of the total population, an uncertainty needs to be attached to the estimate of the concentration of the pollutant. This uncertainty can be related to a distribution model and to its statistical parameters, and a decision is made on the basis of the probability of exceeding a given ecotoxicological threshold. The present study aims at estimating the mean pH of lakes in the southern Québec part of the Canadian Shield, as well as the confidence interval of this estimate using a geostatistical method, considering the autocorrelation structure of the data. Acid precipitation is believed to be the cause of important environmental damage. Wright and Henriksen (1978) were among the first to establish clear links between acid precipitation and regional lake acidification. Following these findings, a maximum 20 kg ha^{-1} $year^{-1}$ target loading of wet sulfate from atmospher-

ic precipitation was proposed by the United States–Canada Work Group (US–Canada 1983) in order to protect moderately sensitive ecosystems. The pursuit of this objective has entailed industrial investments which have contributed to reduce sulfate emissions in the atmosphere. Since that period, governmental agencies have carried out a number of sampling surveys of water chemistry with the purpose of assessing surface water quality and delineating the areas affected by acid precipitation. Surveys of lake chemistry were conducted in the United States (Linthurst and others 1986), in Scandinavia (Henriksen and others 1988) and in Canada (Dupont and Grimard 1986; Kelso and others 1986). Major motivations of these surveys were to delineate areas affected by acidification and to produce data that could be compared to data of the same type to be obtained several years later, in order to establish whether the acid rain control-programs have succeeded in reducing acidity in surface waters. This judgment on the reduction of surface water acidity will be possible only if the amount of uncertainty in the estimation of mean pH is properly quantified. The only ways of improving the estimation are to intensify the sampling or to use more appropriate statistical models.

The geostatistical approach was developed to deal with estimation problems of phenomena presenting a spatial autocorrelation structure among observations. Geostatistical methods use the autocorrelation structure as a deterministic component, to estimate – without bias and with minimum estimation variance – values for points that were not measured, or to estimate average values for new "supports" (surfaces or volumes of different sizes than those of the actual sampling program). Geostatistics has proved very effective for ore reserve estimation in the mining industry (David 1977; Journel and Huijbregts 1978); these techniques are now widely used in several other disciplines such as environmental studies (among others, Posa and Rossi 1991; Schaug and others 1993; Englund and Heravi 1994).

In geostatistics, the spatially structured variation of a phenomenon is quantified by a variogram which describes the degree of dissimilarity between sampling units as a function of their geographical distance. The variogram characterizes the continuity of a random function model describing the spatial dispersion pattern of the study variable. The use of random function models has important practical effects. Taking into account the deterministic aspect of a spatial dispersion allows one to improve the accuracy of estimations in comparison with classical statistical relationships neglecting spatial structures, or to reduce the sampling effort needed to achieve a predetermined degree of precision. The present paper has the objective of providing (1) estimates of the mean pH of lakes and of the proportion of lakes with pH below a reference value, and (2) measures of uncertainty for these estimates. The method is based on a set of simulations of a random function model that capture both the deterministic and random components of the spatial dispersion of lake pH in the study area.

Lake water quality survey

Sampling surveys for water chemistry were carried out by the *Ministère de l'Environnement du Québec* between 1986 and 1990, with the purpose of assessing surface water quality and delineating areas affected by acid precipitation in the most sensitive parts of the Canadian Shield (Fig. 1). Lake-water sampling units were collected from 1239 lakes covering the southern part of the Canadian Shield (Dupont 1991). Sampling was conducted during winter, under ice cover, near the center of each lake. Water sampling units were analyzed for 19 chemical variables including pH. Three sampling units were taken and analyzed from each lake in order to evaluate the data variability due to sampling and laboratory analyses. No significant differences were revealed among sampling units (Dupont 1991). Figure 2 gives the histogram and summary statistics of pH values for the 1239 lakes. A goodness-of-fit Kolmogorov-Smirnov test of normality, including the correction proposed by Lilliefors (1967), established that the distribution of pH values was fairly normal (K-S statistic: 0.0452; P-value ≈ 0.01).

Methods

Classical statistical relationships usually neglect spatial autocorrelation structure and only consider the random component of the spatial process. Generally, if the spatial autocorrelation structure is present and well-developed, the use of geostatistical methods can have important practical effects. It allows one to perform local estimation and to improve the accuracy of estimates. Several geostatistical methods have been developed to compute the confidence interval of an estimate (Journel and Huijbregts 1978; Cressie 1991). Ordinary kriging allows calculation of the error variance related to each estimate. This kriging variance is independent of the data values and depends on the sampling configuration and on a chosen variogram model. It represents the average estimation error variance for a fixed configuration of sampling units. Generally, the estimation errors are assumed to be normally distributed with zero mean, and the kriging variance allows the construction of a symmetrical confidence interval around the estimated value. A major problem is that the error variance is not conditioned by the data, and iso-kriging-variance maps generally only tend to mimic data position maps (Journel 1983).

To overcome these drawbacks, parametric methods such as disjunctive kriging (Matheron 1976), multigaussian kriging (Verly 1983) and bigaussian kriging (Marcotte and David 1985), as well as nonparametric methods such as indicator kriging (Journel 1983) and probability kriging (Sullivan 1984), were developed to estimate the conditional cumulative distribution function of the variable of interest. However, disjunctive kriging and nonparametric methods do not ensure that the cumulative distri-

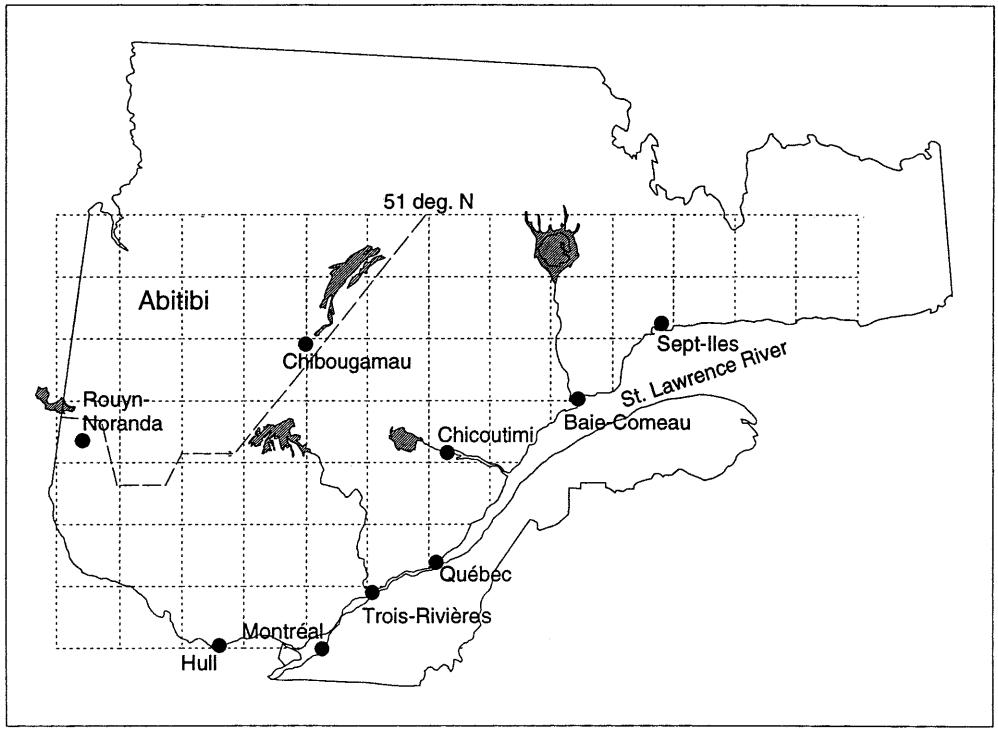

Fig. 1
Location map of the lake water quality survey, south of 51°N and north of St. Lawrence River, in the Québec peninsula, Canada, and delimitation of 100 km × 100 km surfaces for which statistics are computed. The dashed line delimits Abitibi

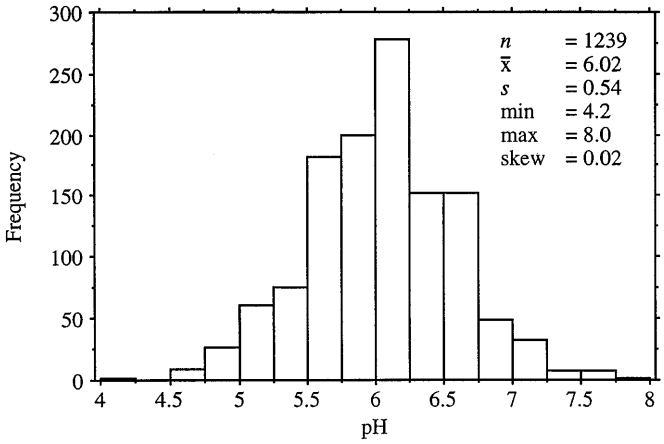

Fig. 2
Frequency histogram of pH values in 1239 lakes of the lake water quality survey; x̄ arithmetic mean, *s* standard deviation, skew = skewness

bution function $F(z) \in [0, 1]$ is non-decreasing. Moreover, for data collected on a point support, inference on surfaces or volumes requires a change of support model. Bigaussian and multigaussian methods do not have inconsistencies in the estimated probability distribution, as opposed to disjunctive kriging and nonparametric methods. Parametric methods, on the other hand, all require bigaussian or multigaussian distributions of normal-transformed variables. This strong hypothesis cannot easily be tested from the data.

As indicated by Englund (1993), conditional spatial simulation is a technique that has great potential as a tool for dealing with various problems associated with spatial uncertainty. Conditional spatial simulation refers to the generation of spatial data constrained to reproduce a given variogram model and the observed values of a pre-existing set of sample data. The use of simulations allows direct extrapolation of probability distributions from point support to any given surface or volume.

Spatial structure and kriging

The variogram is the basic tool of geostatisticians for the estimation and mapping of regionalized variables. It reveals the randomness and the structured aspects of the spatial dispersion. The experimental variogram is defined as:

$$\gamma^*(h) = (2N(h))^{-1} \sum [z(x) - z(x+h)]^2 \quad (1)$$

where $z(x)$ and $z(x+h)$ are measurements of a given variable at locations x and $x+h$, separated by the directional distance h, and $N(h)$ is the number of pairs of sampling units considered in the given distance class. This calculation is repeated for different values of h and provides the experimental variogram which is a plot of the values of $\gamma^*(h)$ as a function of distance h. Generally, the variogram tends to level off at a sill equal to the empirical variance of the variable for large fields relatively to the scale of the autocorrelation structure. The distance at which this occurs is referred to as the range of the variable. The range is the distance over which the sampling sites cease to be spatially correlated. The discontinuity at the origin (non–zero intercept) is called the nugget effect. It is a random component corresponding to the local variation occurring at scales smaller than the sampling interval.

Kriging is a linear-weighted average interpolation technique used to estimate unknown points, surfaces or volumes, from surrounding sampling units. The estimation of a variable $z(x_0)$ at location x_0 is carried out from a combination of the values observed in the surrounding neighborhood ($z(x_1)$, ... $z(x_i)$, ... $z(x_n)$):

$$z^*(x_0) = \sum_{i=1}^{n} w_i \cdot z(x_i) \quad (2)$$

where w_i are the weighting coefficients associated with the sampling values $z(x_i)$ which sum to 1 to ensure unbiased results ($E[z^*(x_0) - z(x_0)] = 0$). The w_i are estimated in such a way as to minimize the variance of errors of estimates.

In the case of ordinary kriging, intrinsic stationarity conditions are assumed, representing conditions of application of the model. They correspond to the hypothesis of a certain regional homogeneity of the spatial dispersion of the phenomenon. If the population mean and the spatial covariance are constant over the study area, the variogram has a sill and the variable under study is said to be second-order stationary. If the variogram does not have a sill, then the covariance does not exist, but kriging can still be performed. This situation corresponds to the intrinsic hypothesis situation.

Conditional simulations

The use of a random function model to describe the spatial dispersion pattern of a phenomenon allows us to perform conditional simulations, where alternative and equally probable high-resolution models of the spatial dispersion of the study variable are generated. Such simulations produce plausible spatial patterns which 'honor' the experimental values (i.e., the real data points with their observed values are among the simulated data) and correspond to the same underlying variogram model. Journel and Huijbregts (1978, chap. 7), Deutsch and Journel (1992, chap. 5) and Dowd (1992) provide the theory for these simulations.

The empirical data and the variogram model have been used to construct several stochastic images of potential lake pH values for a given surface. Post-processing of a large number of these simulations, all equally likely to occur, directly shows the mean value, the probability of exceeding a given environmental threshold, as well as a probability interval for the mean value, for any given surface. The procedure involves the following steps (Fig. 3):

1. Generate a number of simulated point values covering the study area.
2. Define the surfaces over which the mean values are to be calculated.
3. For each simulation, the simulated points falling within a given surface are averaged, giving a simulated local value for the surface $S(x)$.
4. Producing a series of n simulations allows estimation of a prediction interval for the mean of pH and for the proportion of lakes strongly affected by acidification ($pH \leq 5.5$).

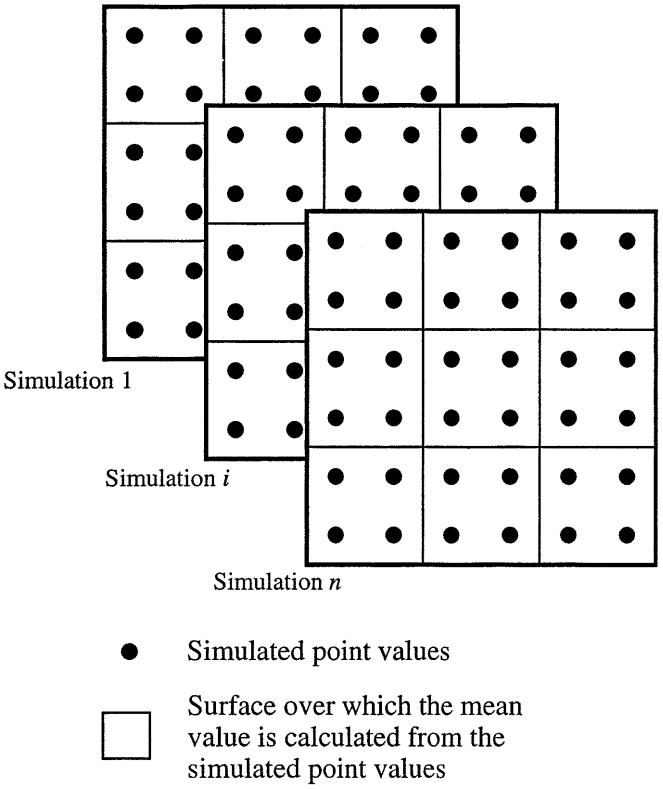

Fig. 3
Calculation method of a probability interval for statistical parameters of given surfaces from conditional simulations. Plausible point pH values are simulated over the whole survey area, and for each simulation, the mean pH value for each surface is calculated by averaging the point pH values falling within a given surface

A sequential Gaussian simulation algorithm found in Deutsch and Journel (1992) was used for these simulations. It consists of the following steps:

1. Transform all data to standard Gaussian values.
2. Calculate and model the variogram of the transformed values.
3. Define a grid of n nodes on which values are to be simulated.
4. Simulate nodes in a random sequence, estimating the value at a given node by kriging, and using a local neighborhood containing all the other values (simulated and experimental).
5. Under the multigaussian hypothesis, at a given grid node, the estimated value (kriged) and the kriging variance are the parameters of a Gaussian distribution. A value is drawn at random from this Gaussian distribution and constitutes a value of the set of simulated data.
6. Go back to step (4) until values have been simulated at all grid nodes.
7. Take the inverse Gaussian transformation used in step (1) to return to the original variable.

Surfaces of 100 km × 100 km containing 36 simulated points arrayed in a 6 × 6 grid have been considered.

Results

Variograms

Figure 4 shows the experimental variograms of the pH values computed for four directions, as well as the fitted model. These directional variograms do not present strong geometric or zonal anisotropy; fluctuations at distances greater than 175 km do not allow the identification of any clear pattern of anisotropy, so they can be considered isotropic. The resulting model can be adequately represented by combining two simple variogram models with different ranges and with their own structured variance components, each one characterizing the variability at a particular scale (Table 1). The global model reaches a sill at a distance of approximately 250 km. The variance of the data (0.2916) is approximately equal to this sill value (0.298). The nugget effect (model 0 in Table 1), corresponding to the amount of random variation in the data, represents 25% of the spatial variation (=0.075/0.298). The nugget effect reflects micro-structures at scales smaller than the sampling interval as well as an integration of the measurement errors.

The structured spatial variation exhibits two structures corresponding to a pronounced increase at small lag distances (0–20 km) and a long-range structure (0–250 km). The global variogram is modeled by the sum of two spherical models (models 1 and 2 in Table 1) and a nugget effect. The global model has the following set of equations:

$$\begin{aligned}
&\gamma(h) = C_0 + C_1\,[1.5(h/a_1) - 0.5(h/a_1)^3] \\
&\qquad + C_2[1.5(h/a_2) - 0.5(h/a_2)^3] \qquad \text{if } h \le a_1 \\
&\gamma(h) = C_0 + C_1 + C_2[1.5(h/a_2) - 0.5(h/a_2)^3] \\
&\qquad \text{if } h > a_1 \text{ and } h \le a_2 \\
&\gamma(h) = C_0 + C_1 + C_2 \qquad \text{if } h > a_2 \\
&\gamma(0) = 0
\end{aligned} \tag{3}$$

where C_0 is the nugget effect, C_1 and C_2 are the structured variance contribution values, a_1 and a_2 are shape parameters which, for a spherical model, give the range of each model, and $C_0 + C_1 + C_2$ is the sill. An important part of the structured spatial variation is related to a regional scale where the zone of influence (range) is approximately 250 km. This structure accounts for 55% (=0.163/0.298) of the total spatial variation. The small-scale model has a range of 20 km and a variance component of 20% (=0.060/0.298).

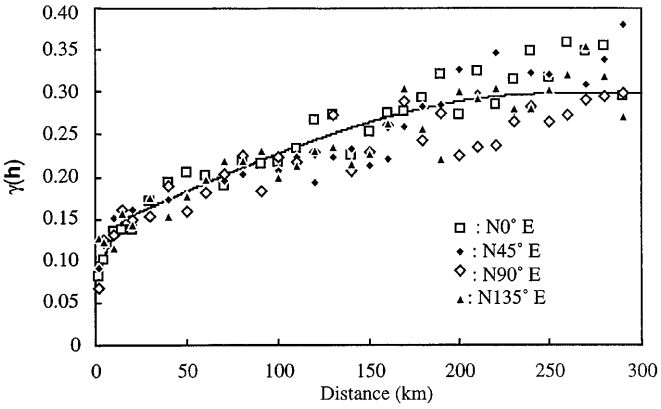

Fig. 4
Directional variograms of pH values in 1239 lakes of the lake water quality survey and spherical variogram model

Table 1
Parameters of nested variogram models for lake pH data and Gaussian transformed scores of pH. C_0 is the nugget effect, C_n is the variance component associated to a given structured spatial scale and a_n is the practical range of the model

Model	Parameters (pH)	Parameters (Gaussian pH)
0. Nugget effect	$C_0 = 0.075$	$C_0 = 0.25$
1. Spherical	$C_1 = 0.060$ $a_1 = 20$ km	$C_1 = 0.21$ $a_1 = 20$ km
2. Spherical	$C_2 = 0.163$ $a_2 = 250$ km	$C_2 = 0.54$ $a_2 = 250$ km

Cross-validation procedure

A cross-validation procedure is used to assess the relevance of the chosen variogram model and to select the best search method – search radius and number of points to use in the kriging system. The search method is chosen on the basis of statistics for the errors, by comparing estimated and observed values. The sampling unit value at a particular location is omitted, and the value at this location is estimated using the remaining neighboring sampling units.

Cross-validation results are presented in Table 2. Each solution reasonably satisfies the global unbiasedness condition, where the distributions of errors ($z^*(x_i) - z(x_i)$) are centered on a zero mean. The spread of the errors given by the standard deviation, and the correlation coefficient of the known values against the kriged estimates, were used to determine an adequate search strategy. On this

Table 2
Cross-validation results of search methodology (search radius and maximum number of points). $\bar{x}_E$ and SD_E are the mean and standard deviation of the error ($z^*(x_i) - z(x_i)$), r and b_1 are the correlation coefficient and the slope of the linear regression $z = b_0 + b_1 \cdot z^*$

Search Radius (km)	Max. nr. of points	$\bar{x}_E$	SD_E	r	b_1
75	8	0.048	0.793	0.61	0.91
75	12	0.039	0.797	0.61	0.92
100	8	0.042	0.794	0.61	0.91
100	12	0.031	0.786	0.64	0.95
150	12	0.031	0.789	0.64	0.95
150	16	0.033	0.776	0.67	0.98
250	16	0.032	0.778	0.70	0.99
250	24	0.032	0.775	0.71	0.99
300	30	0.031	0.777	0.71	0.99

basis, a search radius of 250 km and the use of the nearest 24 points were selected as an optimal solution. The estimation procedure performed better for large radii and high numbers of points, showing that the long-range structure contributed to the estimation. Notice that the slope of the regression coefficient b_1 [of $z(x_i)$ against $z^*(x_i)$] is close to but always smaller than one. It indicates that the kriging procedure slightly underestimated the true low values, and overestimated the high values.

Conditional simulations

The probability distributions of pH values in given surfaces S(x) are estimated through the realization of numerous small-scale conditional simulations of normal scores of pH performed on a dense grid of points. The normal scores of simulated point values were backtransformed to obtain pH values. The pH values were averaged over a surface S(x), providing a simulated mean pH for a surface. In order to obtain the proportion of lakes affected by acidification, each normal score of point values was transformed to pH values. The proportion of affected lakes was directly estimated by the number of pH point values less than or equal to 5.5, divided by the total number of simulated points in the surface S(x) (Fig. 5b). A pH of 5.5 was considered as the threshold value because at this pH, it is recognized that adverse environmental effects are produced affecting many organisms in aquatic systems (Schindler 1988). A histogram of simulated values was constructed; the mean and the prediction interval limits were computed directly from the frequency distribution for predetermined quartile limits. For example, Fig. 5a indicates that, for a surface of 100 km × 100 km around Rouyn-Noranda, the lower and upper 95% predictive limits for the mean pH are 5.78 and 6.36. Because a number of possible mean values for given surfaces have been simulated, it is therefore possible to estimate the local spatial probability of exceeding a given critical level by directly reading on the histogram the quartile corresponding to the threshold. For example, Fig. 5a shows that the probability, for the mean of lake pH to be <6.0, is 0.272.

Generally, classical statistical relationships are used to calculate a confidence interval for the mean and the proportion of affected lakes. Figure 6 shows the relationships between 95% confidence intervals deduced from usual classical relationships and 95% prediction intervals deduced from conditional simulations. The comparison of these methods is done by using the variance of the total sample of 1239 lakes ($s_X^2 = 0.29$) and the relationship $s_{\bar{X}}^2 = s_X^2/n$ to estimate the uncertainty associated with the estimation of the mean pH for surfaces of 100 km × 100 km (Fig. 6a). The value of n represents the number of sampling units in a surface of 100 km × 100 km. This comparison integrates regional information on the total population, and it supposes the homogeneity of the phenomenon and the absence of spatial autocorrelation in the data. Figure 6a shows that the prediction intervals calculated from geostatistical simulations are generally smaller than confidence intervals and

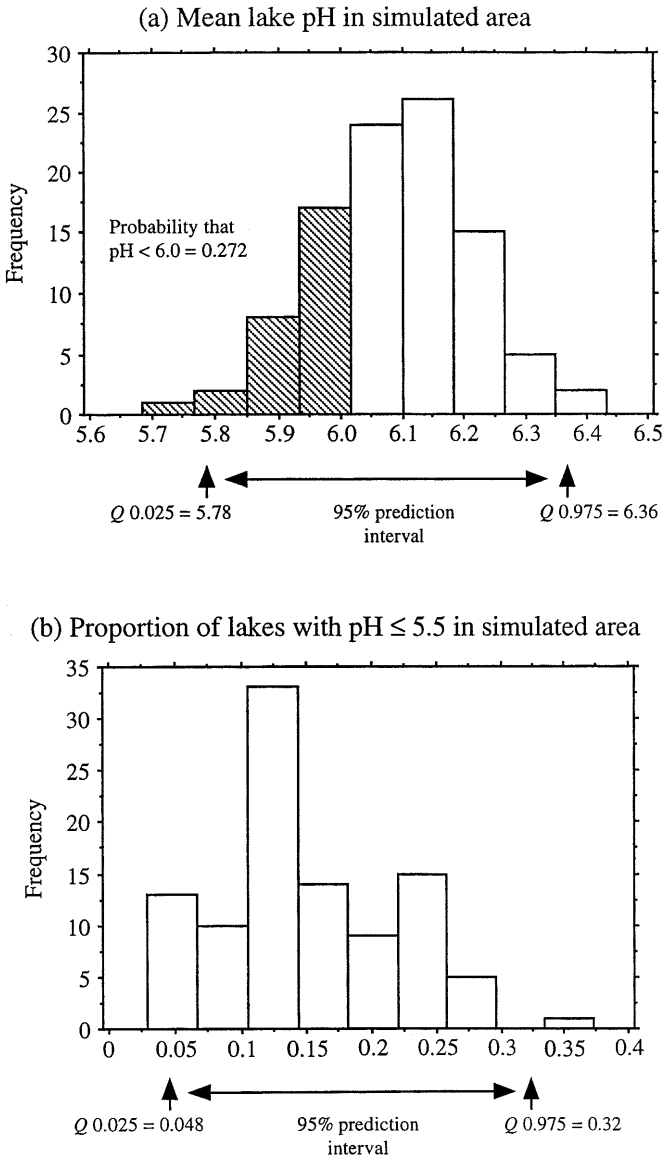

Fig. 5
Results of repeated simulations over a small area (100 km × 100 km) around Rouyn-Noranda. **a** Frequency distribution of the mean, over the small area, of the simulated lake pH values. **b** Frequency distribution of simulation results distributed according to the proportion of lakes with pH ≤ 5.5 (abscissa). Quantiles (Q) are used to estimate probabilities and prediction intervals

are relatively constant for all surfaces. Prediction intervals deduced from conditional simulations range from 0.25 to 0.8 pH unit, while confidence intervals deduced from classical relationships range from 0.25 to 3.8 pH units. These results demonstrate that it is difficult to calculate local probabilities with the few sampling units contained in surfaces of 100 km × 100 km. Figure 6b shows prediction intervals versus confidence intervals for the proportion of lakes with pH ≤ 5.5. A group of points, spread out along the line of slope 1, indicates equivalent intervals for all methods. However, a group of points lo-

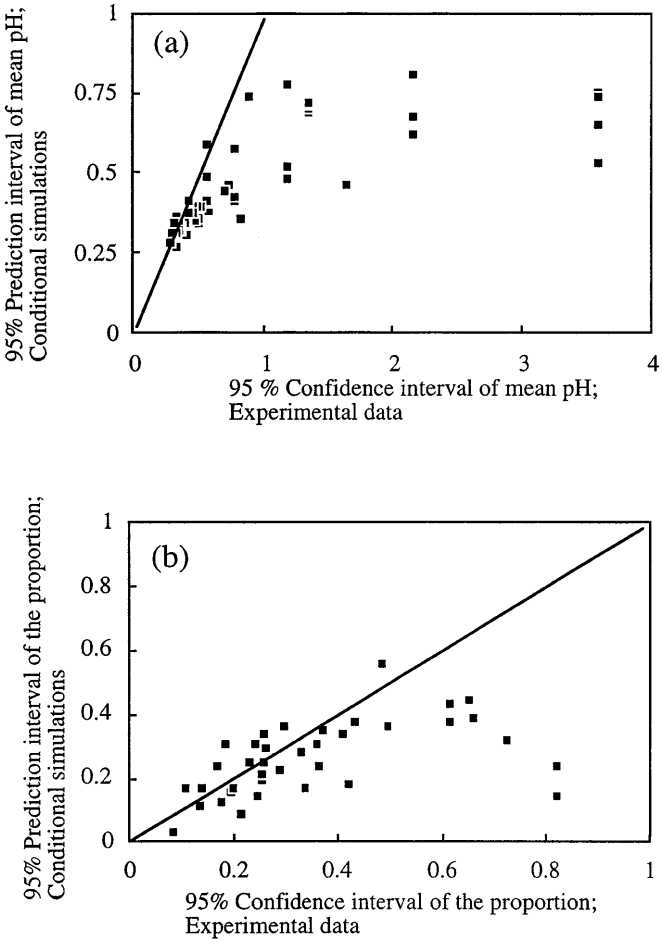

Fig. 6
Relationship between 95% confidence intervals deduced from classical statistical relationships and prediction intervals for (**a**) mean of pH using information about the whole sample of 1239 lakes, (**b**) proportion of lakes with pH ≤ 5.5. The line of slope 1.0 is shown as reference. A 100(1–α)% symmetrical confidence interval for the mean is given by $I = 2 \cdot t_{\alpha/2} \cdot s_{\bar{x}}$, where $s_{\bar{x}}$ represents the standard deviation of the sample mean ($s_{\bar{x}} = (s_x^2/n)^{0.5}$), and $t_{\alpha/2}$ is the (1–α/2) quantile of the Student t distribution. An approximate 100(1–α)% symmetrical confidence interval for a proportion p is given by $I = 2 \cdot t_{\alpha/2} \cdot (\mathrm{var}(p^*))^{0.5} + (1/2n)$, where

$$\mathrm{var}(p^*) = \left(\frac{N-n}{N}\right) \frac{p^*(1-p^*)}{n-1},$$

n is the sample size and N is the population size

cated under the line presents large confidence intervals when there are few sampling points in the surfaces ($n < 15$).

Conditional simulations, which consider a spatial autocorrelation model linking together the observations, lead to an improvement of the precision of estimates and allow estimation within regions that contain little information. If a surface contains several sampling units, the simulated points are strongly conditioned by these sampling units; and the high sampling density and the small-scale correlation structure ensures low kriging variance. As a consequence, the simulated values are drawn from a narrow distribution, providing a small confidence interval for the mean. On the other hand, if a surface contains few sampling units, then the surrounding regional information and the regional autocorrelation structure contribute to the estimation of surfaces with little information. It should be noted that simulations can represent the reality only if the variogram model also represents the reality. Considering the shape of the experimental variogram, it clearly indicates that the spatial dispersion of pH values is not random, but spatially structured. Moreover, each experimental variogram value is calculated using more than 164 pairs of sampling points, providing a good confidence in the chosen variogram model.

The calculation of mean values and prediction intervals was done for the whole survey area. It allowed us to map the estimated mean values and probability of exceeding a given threshold to determine the areas affected by acidification. The prediction intervals of each surface can also be mapped to point out the areas displaying the largest estimation errors which can be due to low sampling density or to an unfavorable sampling configuration (Figs. 7 and 8).

The Abitibi area, in the region of Rouyn-Noranda, is strongly affected by lake acidification (Fig. 7a). This area is an important mining district and is subjected to smelter emissions. Moreover, sulfide minerals contained in ore deposits and associated rocks have been spread by glaciers and can make up an important component of glacial deposits, representing a natural source of acidity (Shilts and others 1981). Bedrock, soil and surficial sediments of this area have a low capacity to neutralize acid solutions. Low pH are also found in the Baie-Comeau-Chicoutimi area. This area is characterized by granite gneiss lithologies overlain by a very thin soil cover derived from local bedrock, producing a sensitive cover to acid loading with low buffering capacity.

High pH found south and east of Chibougameau (3 white squares in Fig. 7a) are associated with carbonate-rich glacial material. This type of glacial deposit is also found north of Rouyn-Noranda, reducing the effect of sulfate emissions. Similarly, high pH in the Montréal-Hull area correspond to the occurrence of limestone and fine-grained glacio-marine and glacio-lacustrine sediments with an important buffering capacity produced by the process of cation exchange and hydrolysis (Shilts and others 1981).

Figure 7b shows that the highest uncertainties of pH estimates occur in the periphery of the study area where few experimental points are involved in the estimation procedure, and in the region north of Rouyn-Noranda where few lakes can be sampled due to low lake density.

Figure 7c shows that the simulation model allows the calculation of the spatial probability of exceeding a given threshold. The general spatial pattern is similar to the spatial pattern of local mean pH. It shows that the probability for the mean pH to be ≤ 6.0 reaches 1.0 two squares east of Rouyn-Noranda and in the Baie-Comean area.

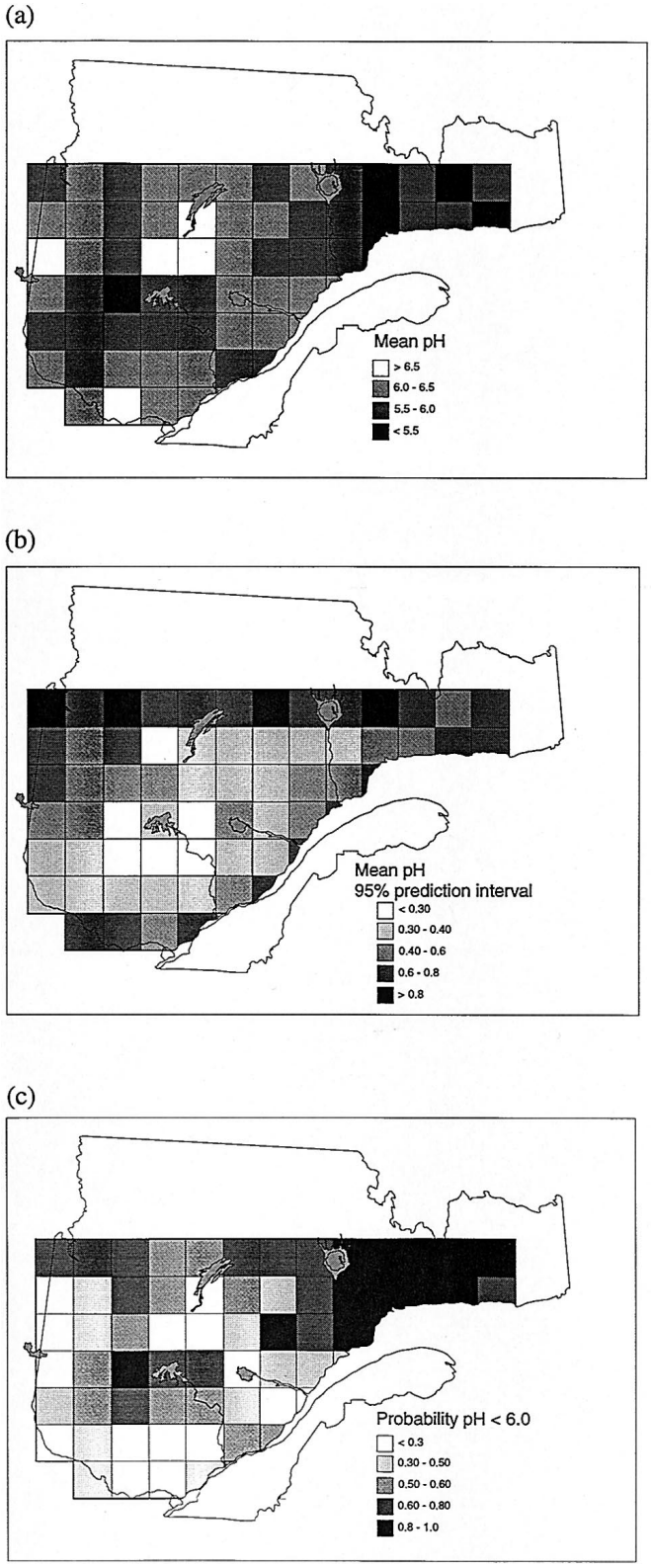

Fig. 7
Estimated mean values and 95% prediction intervals for mean of pH, calculated over surfaces of 100 km × 100 km (conditional simulations for b and c)

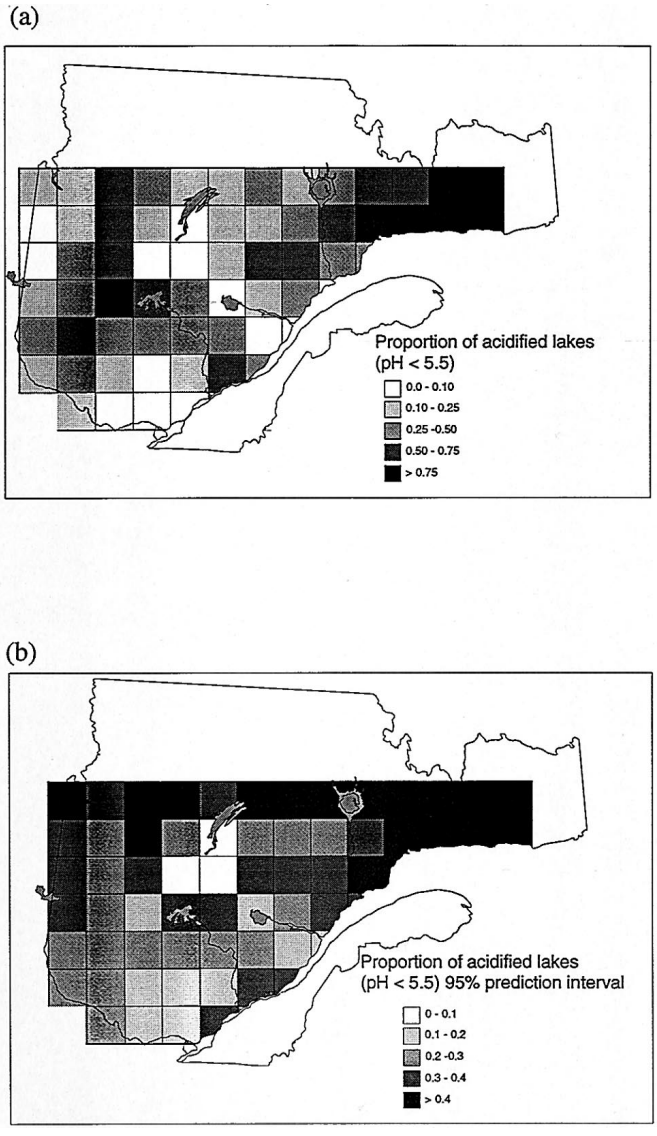

Fig. 8 Estimated mean values and 95% prediction intervals for proportion of lakes with pH ≤ 5.5, calculated over surfaces of 100 km × 100 km (conditional simulations)

One of the fundamental goals of lake water quality surveys is to obtain interval estimates of the number of lakes in defined geographic regions that may be sensitive to acid deposition (Patil and others 1985; Dupont 1991). This estimate is a direct measure of the extent of the acidification problem. Simulations allow the direct calculation of this type of statistic. The general spatial dispersion pattern of this variable (Fig. 8a) and its prediction interval (Fig. 8b) are very similar to the dispersion of mean pH and its prediction interval. Figure 8a shows that locally, the proportion of lakes strongly affected by acidification can exceed 50% in surfaces of 100 × 100 km in the Abitibi and Baie-Comeau areas. For Abitibi, Dupont (1993) reached very different conclusions. He concluded that 16% of the lakes have a pH ≤ 5.5, with lower and upper confidence limits of 11.79% and 21.02%. This area,

delimited on Fig. 1 (dashed line), covers approximately 155 000 km^2. This regional estimate gives a poor picture of the situation. The important difference in the estimates of the proportion of lakes strongly affected by acidification is due to two main factors. First, Dupont (1993) performed estimation over a large area while our estimation used much smaller surfaces. There is important small-scale heterogeneity between small areas, which is not taken into account when considering a large drainage basin. Geological and pedological features present small-scale variation in this area. Second, the model used by Dupont (1993) considers a random spatial pattern, while our model integrates structured spatial variation.

Conclusion

The assessment of uncertainty is a central problem in environmental evaluation. The evaluation of potential errors of estimation constitutes a key information to appreciate the seriousness of an environmental problem. A conditional simulation procedure has been applied to estimate local means, probabilities and confidence intervals of pH values. The method allowed the production of accurate local pH estimates enabling the delimitation of areas affected by lake acidification. Conditional simulations of a random function model, taking into account the spatial autocorrelation structure of the data, produced more accurate estimates than estimation based upon classical statistical relationships, showing the usefulness of the deterministic component of the model.

The southern part of the Canadian Shield in Québec shows large geographical variation in lake acidity. Two areas are identified as strongly affected by lake acidification. The area east of Rouyn-Noranda is subjected to smelter emissions; bedrock and mining activities represent additional sources of acidity in this area. The Baie-Comeau area is characterized by lithologies and a thin soil cover with low buffering capacity. In return, some large areas display high pH values due to high buffering capacity related to the occurrence of carbonate-rich material in bedrock and glacial deposits, or the occurrence of clay deposits.

Previous studies on lake acidity using classical statistical relationships have drawn conclusions at the scale of large drainage basins (Dupont 1991), neglecting small-scale phenomena acting as local sources of heterogeneity. These sources of heterogeneity produce sharp transitions between affected areas and other areas with high buffering capacity. This phenomenon is particularly obvious in the Abitibi and Baie-Comeau areas, where changes in physiographic features produce changes in pH levels. These sharp transitions are taken into account by the small-scale structure of the variogram. Generally, few sampling units are available in a small region, making it difficult to estimate a local pH value. One of the major advantages of the conditional simulation technique is its ability to produce accurate local estimates with a potential error determined by sampling density and configuration, data values and autocorrelation structure. The estimation of accurate local values with low potential errors allows a more precise evaluation of the extent of environmental problems.

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