

Visualizing Spatial Uncertainty of Multinomial Classes in Area-class Mapping

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Abstract: Area-class maps are conventionally delineated by human hands based on limited observed (or high-quality) data and expert knowledge. It is recognized that area-class maps contain spatial uncertainty because the classification of unobserved locations is not completely certain. Spatial uncertainty associated with an area-class map may be quantified by spatial statistical approaches through estimating the occurrence probability of a class at each unobserved location. In this study, we use both indicator kriging and the recently proposed Markov chain geostatistics (MCG) to simulate spatial distribution of multinomial classes and assess spatial uncertainties associated with simulated results. The spatial uncertainties are represented by occurrence probability vectors, which are further visualized as occurrence probability maps. Results show that given the same observed dataset the spatial uncertainty assessed by MCG is apparently lower than that assessed by indicator kriging. In simulated realizations, MCG generates apparently higher PCCs (percentages of correctly classified locations) than indicator kriging. It is concluded that the spatial uncertainty assessed by MCG should be closer to the real spatial uncertainty associated with an area-class map.

1. Introduction

Many spatial variables (e.g., soil distribution, land cover) are classified into multinomial classes and delineated as area-class maps. The delineation of area-class maps may be conducted by human hands or by quantitative methods based on limited observed (or high-quality) data and expert knowledge. While observed data must be honored in map creation, expert knowledge is normally incorporated into human mental qualitative models (for hand delineation) or into parameter estimation of quantitative (e.g., statistical) prediction methods. It is widely recognized that area-class maps created in such ways contain spatial (or locational) uncertainty because the classification of unobserved locations is not completely certain, particularly at the locations of polygon boundaries (e.g., Goodchild and Dubuc 1987, Goodchild et al. 1992, Lagacherie et al. 1996, Lark and Bolam 1997, MacEachren 1992, Mark and Csillag 1989, Wilson and Burrough 1999).

Although interpolation methods can be used to predict the spatial distribution of variables, interpolation, however, does not estimate spatial uncertainty. An interpolated map is not a reflection of the reality because of the smoothing effect. Conditional simulation (i.e., stochastic imaging) provides an alternative to interpolation in which both original data and the statistics of the original data are honored. The word “*conditional*” refers to the fact that simulated values take into account original data and previously simulated data. Thus, conditional simulation produces maps in which the general patterns of spatial variation in the original data are recreated, and which, consequently, are “*possible realities*”. The multiple realizations generated by conditional simulation embody the inherent uncertainty in the original spatial samples (Curran and Atkinson 1998). And more interestingly, we may estimate the occurrence probabilities of single classes at every location – probability vectors - from a number of simulated realizations as the complete estimates of spatial uncertainty.

Probability vectors were suggested to represent the spatial uncertainty of categorical variables (Goodchild et al. 1992, Mark and Csillag 1989) and they can be further visualized as a series of probability maps to demonstrate spatial uncertainty of classes at each location of the

mapped area (Li et al. 2005, Zhang and Li, 2005). However, the acquirement of accurate probability values for representing spatial uncertainty depends on the development of high quality stochastic conditional simulation models, and adequate models for assessment of spatial uncertainty of area-class maps have been lacking (Goodchild 2003; MacEachren et al. 2005). An area-class map is a collection of discrete objects (i.e., polygons). In repeated mappings, positions and numbers of objects may vary and positional uncertainties widely depend on boundary clarity. Goodchild (2003) suggested six requirements of error (i.e., uncertainty) models for area-class maps: (1) the model should address confusion at every point between observed class C' and consensus class C ; (2) variation between realizations should emulate variation between repeated mappings; (3) autocorrelations should be incorporated in outcomes at nearby points; (4) the model should emulate effects of map generalization, both thematically and cartographically; (5) realizations should be invariant under changes in underlying representation, e.g., raster cell size; and (6) in nominal case simulated results should be invariant under reordering of classes. He further examined six models ever suggested for error modeling of area-class maps and pointed out their pros and cons. We think it may be useful to consider two extra requirements: (1) interclass relationships should be respected and (2) the model should deal with classes nonlinearly.

In visualizing spatial uncertainty, MacEachren (1992) suggested three methods: (1) map pairs in which a data map is depicted side-by-side with a map of uncertainty about that data; (2) sequential presentation in which a user might be warned about uncertainty with an initial map which is followed by a map of the data (or interactive tools that allow toggling between the data and the uncertainty representations); and (3) bi-variate maps in which both the data of interest and the uncertainty estimate are incorporated in the same map. With probability vectors the map-pair strategy may be expanded into a map-series strategy, which includes a map of the data, a map of uncertainty for the data map, and a series of maps of uncertainty for single classes (Li et al. 2005, Zhang and Li 2005). Most attempts thus far to graphically depict uncertainty of spatial data have used the map-pair (or -series) strategy, partly maybe because this strategy is intuitive and easy to present (e.g., Bierkens and Burrough 1993, Zhang and Goodchild 2002).

Conventional geostatistical methods are widely used to deal with the uncertainty of continuous variables. However, methods for simulating and assessing uncertainty of categorical variables are relatively rare. As a practical spatial statistical technique for prediction and conditional simulation of indicator variables (cutoffs and thresholds of continuous variables, and categorical variables), indicator kriging geostatistics is commonly cited as a potential candidate for spatial uncertainty assessment of categorical variables (e.g., Goovaerts, 1997) and has been used for spatial uncertainty analysis of categorical variables in pioneer studies in the last decade (e.g., Bierkens and Burrough 1993, Kyriakidis 2001, Zhang and Goodchild 2002). However, conventional indicator kriging geostatistics such as the popularly used sequential indicator simulation (SIS) algorithm has limitations such as using linear estimators (Bogaert 2002) and only considering spatial auto-correlations. Currently, it still has difficulties to incorporate interclass relationships into indicator kriging algorithms. Thus, they use only part of spatial heterogeneity information conveyed by data and expert knowledge and deviate from experts's human mental models, which are normally nonlinear and consider interclass relationships and ancillary information in delineating an area-class map. The recently-proposed Markov chain geostatistics (MCG) is a new emerging spatial statistical approach outside kriging, specifically suggested for prediction and conditional simulation of multinomial classes (Li and Zhang 2005b). Methodologically, MCG is closer to human mind of experienced experts in estimating

an unobserved location because of its nonlinearity and incorporation of interclass relationships. Thus, this approach may better capture spatial patterns of multinomial classes at their approximate locations and generate less spatial uncertainty.

In this study, we use both indicator kriging geostatistics and MCG to assess spatial uncertainties associated with area-class maps through conditional simulations. The spatial uncertainties are represented by occurrence probability vectors, which are estimated from simulated results and further visualized as occurrence probability maps. We use both simulated realizations and occurrence probability maps generated by the two approaches to show the spatial uncertainties that may exist in area-class mapping. By comparing results generated by the two approaches we show that MCG has some advantages over indicator kriging geostatistics for estimating spatial uncertainty of area-class maps. Since we focus on visualizing the spatial uncertainty of multinomial classes in area-class mapping, the technical details of MCG and indicator kriging will not be introduced in this paper.

2. Area-class Mapping

In making area-class maps, the traditional method is hand-delineating based on field survey data and expert knowledge of surveyors. Most existing area-class maps, such as the United States Department of Agriculture Soil Survey Geographic Database, were created in this way. The development of modern geostatistics provides the possibility of automatic area-class mapping. Below we examine the processes of creating an area-class map using different ways.

2.1. Hand-delineating

In hand-delineating an area-class map, map creators need to use the following information: (1) observed data, which may be observed points or other styles of data, (2) expert knowledge, which may be built on domain knowledge and field/lab experience, and (3) if available, ancillary information such as topographical data, as illustrated in Figure 1. The observed data (assumed correct) must be honored in the mapping process. Based on the observed data, their domain knowledge and field experience, and available ancillary information, map creators build their expert knowledge about the mapped area and map classes, which may include class number and names, approximate proportion of each class, general polygon size of each class (i.e., autocorrelation), spatial configuration of different classes (interclass relationships), etc. Based on the expert knowledge, map creators further build their mental qualitative models for mapping the classes. Although no specific spatial measure is used, both autocorrelations and interclass relationships (e.g., cross-correlations) are more or less qualitatively included in their mental models.

Autocorrelation can be embodied on polygon sizes of single class points or the boundary location between two observed points with different class labels. For example, if map creators know that class A usually occurs as small polygons (i.e., weakly auto-correlated), when finding a single observed point of class A they may draw a small polygon around the point (Figure 2a); on the contrary, if they know class B usually occurs as large polygons (i.e., strongly auto-correlated), a large polygon will be drawn around a single point of class B (Figure 2b). To decide the class label of an unknown location, map creators actually consider all surrounding observed data, not just those belonging to the same class. This means interclass relationships are considered more or less. For example, assuming there are two neighboring observed points belonging to two different classes, if map creators know that they usually occur as neighbors, the polygons of the two classes will share a common boundary (Figure 2c); otherwise if map

creators know that the two classes can never be neighbors, they will probably draw a strip of class *C*, which is known a neighbor of both class *A* and class *B* (Figure 2d). In addition, mental models of map creators are normally nonlinear because human brains are very complex and do not necessarily consider things linearly.

In addition, if a minor class is missed in sampling but surveyors or map creators can confirm its existence at some places, they also can draw that class on the area-class map.

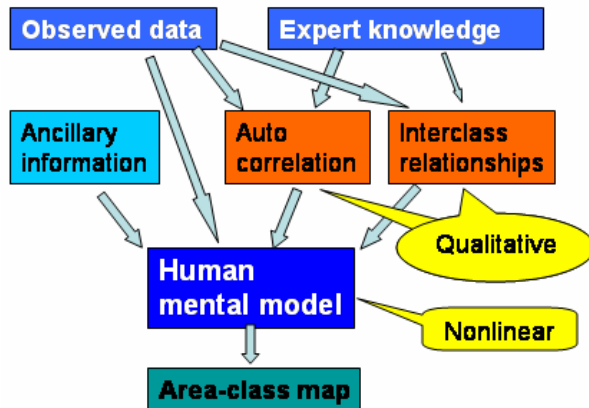


Figure 1. Illustrating how an area-class map is hand-delineated.

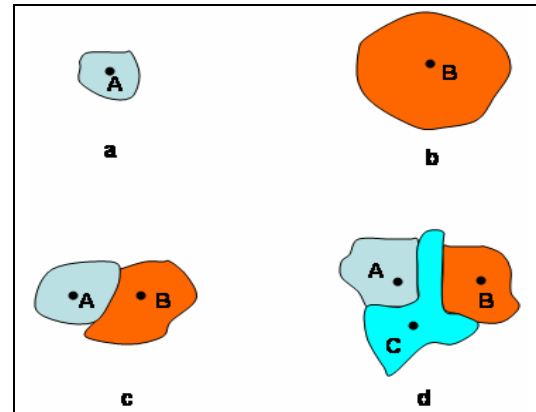


Figure 2. Consideration of autocorrelations and interclass relationships in area-class mapping: **a**, weak autocorrelation; **b**, strong autocorrelation; **c**, classes *A* and *B* are neighbors; **d**, classes *A* and *B* are not neighbors, but both are neighbors of class *C*.

2.2. Indicator Kriging Geostatistics

Indicator kriging was developed for estimating thresholds of continuous variables such as mineral contents. It has been used for interpolation and simulation of categorical variables and in recent year for spatial uncertainty analysis (e.g., Kyriakidis 2001). The most popularly used simulation algorithm of indicator kriging is the SIS algorithm with ordinary kriging (Note that simple kriging is generally inferior to ordinary kriging). In using indicator kriging to interpolate or simulate categorical variables, classes were estimated one by one: when class *A* is estimated, data of class *A* are coded as 1 and other data are coded as 0; and when class *B* is estimated, data of class *B* are coded as 1 and other data are coded as 0. Thus, only observed data of the same class and auto-correlation information of the class are used to estimate the occurrence probability of the class at an unobserved location (Figure 3). Auto-correlation was represented by indicator auto-variogram models (see Figure 4). In modeling experimental auto-variograms estimated from samples, some expert knowledge on auto-correlations such as auto-correlation ranges may be incorporated. Because interclass relationships are completely ignored in SIS, data of other classes do not contribute to the occurrence of the class to be estimated at an unobserved location. Note that theoretically SIS may consider cross-correlations by using cokriging, but in practice it is difficult and no literature can be found. Of course, minor classes missed in sampling will never be captured in SIS. Therefore, SIS did not use all spatial variation information conveyed by samples and expert knowledge. In addition, as an estimator, indicator kriging is still linear (see arguments in Bogaert 2002).

The ordinary indicator kriging estimator for the occurrence probability of a class C_i at the location x_0 is defined as a linear combination of the surrounding indicator data I_α (Cressie 1993), with

$$\Pr(x_0 | x_{i_\alpha}) = \sum_{\alpha=1}^n \lambda_{i_\alpha} I_{i_\alpha}, \quad (1)$$

where the set of weights λ_{i_α} are obtained by solving a system of linear equations

$$\begin{cases} \sum_{\alpha=1}^n \lambda_{i_\alpha} \gamma_{ii}(h_{\alpha\beta}) + \mu_i = \gamma_{ii}(h_{\beta 0}) \\ \sum_{\alpha=1}^n \lambda_{i_\alpha} = 1 \end{cases}. \quad (2)$$

In Equations (1) and (2), $\gamma_{ii}(h_{\alpha\beta})$ denotes the indicator auto-variogram between data locations x_α and x_β , and $\gamma_{ii}(h_{\beta 0})$ denotes the indicator auto-variogram between data location x_β and x_0 ; μ_i is the Lagrange parameter. Apparently, as an estimator, indicator kriging is still linear.

It should be noted that while optimal prediction maps based on maximum occurrence probabilities generated by SIS can be regarded as area-class maps, realizations generated by SIS actually contain only dispersed patterns. To make area-class maps from realizations, one has to delineate polygons further on simulated patterns, which causes a new source of spatial uncertainty.

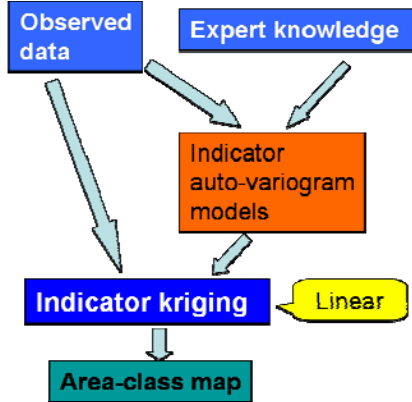


Figure 3. Illustrating the generation of area-class maps using indicator kriging.

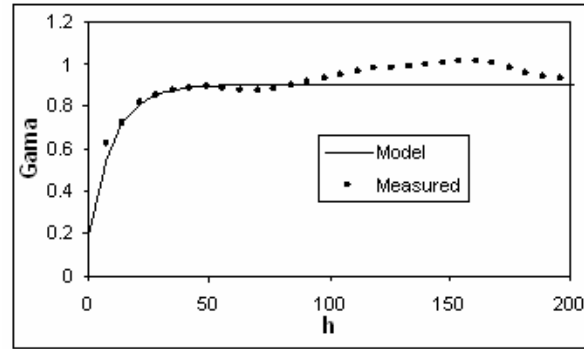


Figure 4. An indicator auto-variogram (experimental data and model).

2.3. Markov Chain Geostatistics

MCG is proposed for dealing with multinomial classes. Compared with indicator kriging, the major advantages of MCG lie in its ability of incorporating interclass relationships and the nonlinearity of its estimator (Figure 5). MCG estimates all involved classes simultaneously. In estimating a class, it considers surrounding nearest data no matter which class they belong to; that is, contribution of data of the same classes to the occurrence probability of the class being estimated is taken into account through auto-transiogram models and contribution of data of other classes is taken into account through cross-transiogram models (Figure 6). For MCG, the modeling of transiograms is far more flexible than the modeling of indicator variograms for

indicator kriging (Li 2006a). If experimental transiograms are reliable, experimental transiograms (discontinuous points) can be directly interpolated into continuous models for simulation (Li and Zhang 2005a). Not only more heterogeneity information conveyed by sample data can be incorporated into simulated results through transiograms, expert knowledge in interclass relationships and classes missed in sampling also can be incorporated into a simulation.

The MCG estimator for the occurrence probability of a class C at the location x is defined as a non-linear combination of the surrounding data (Li 2006b), with

$$\Pr(X(x) = k \mid X_1(x_1) = l_1, \dots, X(x_m) = l_m) = \frac{\prod_{i=2}^m p_{kl_i}^i(h_i) \cdot p_{l_1 k}^1(h_1)}{\sum_{f=1}^n \left[\prod_{i=2}^m p_{fl_i}^i(h_i) \cdot p_{l_1 f}^1(h_1) \right]}, \quad (3)$$

where any $p_{lk}^i(h)$ denotes a transiogram from state l to state k over the lag h in the i th direction, and m is the number of data considered in different cardinal directions.

As a nonlinear geostatistics, a special characteristic of MCG is that it directly generates polygon features in simulated realizations. This does not mean it generates objects directly and ignores inner-polygon spatial uncertainty. In fact, MCG still conducts a simulation pixel by pixel. However, because the patterns generated by MCG are normally strongly convergent, they appear as polygons. Therefore, in area-class mapping MCG is apparently superior to indicator kriging and it is closer to human brains.

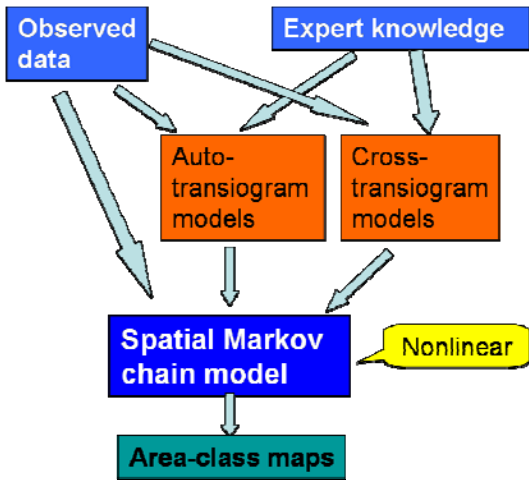


Figure 5. Illustrating the generation of area-class maps using Markov chain geostatistics.

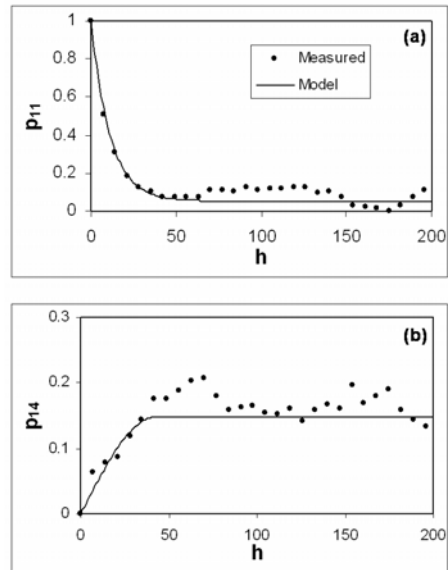


Figure 6. An auto-transiogram (a) and a cross-transiogram (b) (measured data and models).

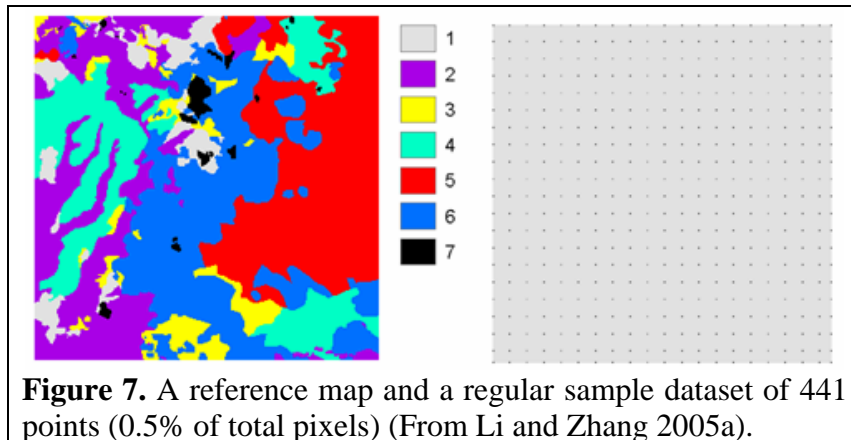


Figure 7. A reference map and a regular sample dataset of 441 points (0.5% of total pixels) (From Li and Zhang 2005a).

3. Spatial Uncertainty Quantification and Visualization

Given a sample dataset, one way to quantify spatial uncertainty associated with unsampled locations is to estimate the occurrence probability vectors of classes at each location from a large number of simulated realizations generated by a

stochastic spatial statistical model. Figure 7 shows a reference area-class map and a sample dataset (Li and Zhang 2005a). The reference map is delineated based on detailed survey and high resolution remote sensing satellite images and we assume it is correct here. The sample dataset is extracted from the reference map. We used both SIS with ordinary indicator kriging and a MCG algorithm to simulate 100 realizations on the dataset, respectively.

Occurrence probability vectors were estimated from 100 realizations for each simulation and visualized as occurrence probability maps. Based on maximum occurrence probabilities, optimal prediction maps (area-class maps) were generated. To show the difference in spatial uncertainty assessment between indicator kriging and MCG, we obtained probability difference maps by subtracting probability values generated by SIS from those generated by MCG.

3.1. Optimal Prediction Maps and Associated Spatial Uncertainty

Figure 8 shows optimal prediction maps generated by the two approaches and their corresponding maximum occurrence probability maps. Apparently, the two prediction maps look quite similar. However, this does not mean that both maps have similar spatial uncertainty. The maximum occurrence probability maps corresponding to these two optimal prediction maps are obviously different. The maximum occurrence probability map from MCG has clearer and narrower white-grey stripes (called transition zones) and darker areas (i.e., polygons) than that from SIS has. The average maximum occurrence probability values from MCG and SIS are 0.883 and 0.749, respectively; the former is 0.134 higher than the latter. It can be concluded, therefore, that the optimal prediction map from MCG is generally more credible (i.e., has less spatial uncertainty) than that from SIS.

Figure 9 displays the difference map of the two maximum occurrence probability maps (i.e., MCG data – SIS data). It can be seen that within polygons, particularly at the places that are close to boundaries (see the dark blue in Fig. 9), MCG generates higher maximum occurrence probabilities than SIS does. But on polygon boundaries (i.e., the transition zones), MCG generates lower maximum occurrence probabilities than SIS does (see the red in Fig. 9). These imply that locations of polygons are more certain in simulated results by MCG than in simulated results by SIS, thus MCG is more desirable in area-class mapping.

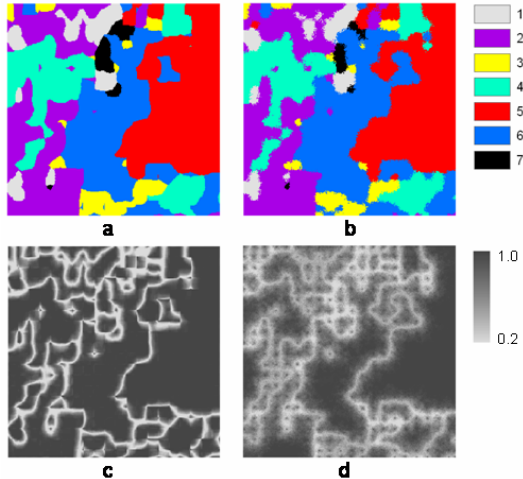


Figure 8. Optimal prediction maps based on maximum occurrence probability maps and corresponding maximum occurrence probability maps, generated by MCG (a, c) and SIS (b, d).

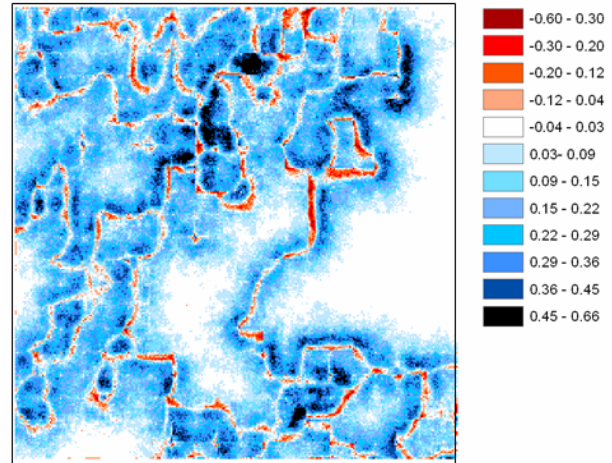


Figure 9. The difference map of maximum occurrence probabilities generated by MCG and SIS (i.e., Difference = MCG data – SIS data).

3.2. Simulated Realizations

Optimal prediction maps contain smoothing effect; for example, small classes may be underrepresented because of their relative lower occurrence probabilities at most locations; hence optimal prediction maps usually do not reflect effectively the complex spatial distributions of classes. In applications, particularly for studying error propagation or for getting the spatial uncertainty information of response variables, it is necessary to directly use simulated realizations as input data or reference data. A single realization represents one possible spatial distribution configuration of classes. Different realizations normally share similar spatial statistics but are more or less different in details. Therefore, spatial uncertainty may also be represented by a number of realizations.

Figure 10 shows two realizations simulated using MCG and two realizations simulated using SIS. Difference in details can be seen from different realizations simulated by the same method. Apparently the two different methods generated different styles of realizations. MCG directly generates polygon maps, which is close to hand-delineated area-class maps. But SIS generates realizations with dispersed patterns, which need further processing to generate polygon maps. While it is difficult to say which kind of realization maps is better, important is the accuracy of a realization in reflecting the real spatial distribution of classes. Using the reference map as verification data, PCC (percentage of correctly classified locations) values were calculated. The average PCC value for realizations of MCG is 75.23% and that for realizations of SIS is 68.51%. So the former is obviously higher than the latter with an absolute difference of 6.72%, which means that MCG can better capture classes at their correct locations. Therefore, it can be concluded that MCG is superior to SIS in simulating multinomial classes.

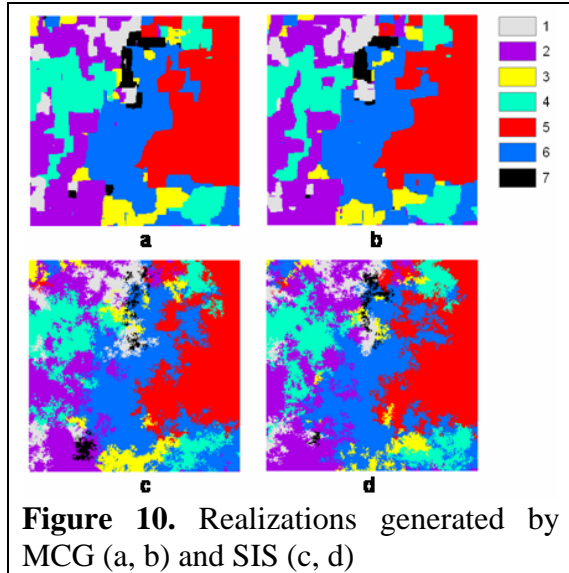


Figure 10. Realizations generated by MCG (a, b) and SIS (c, d)

In the simulation example, because we have no class missed in sampling and also no classes that cannot be neighbors, we cannot examine clearly the differences of the two approaches in obeying the non-neighboring interclass rule and capturing missing classes. But from their different working principles, it is easy to understand the differences of the two approaches in these aspects.

3.3. Spatial Uncertainty of Single Classes

Maximum occurrence probability maps only show the spatial uncertainty or credibility of optimal prediction maps. To effectively represent the spatial uncertainty of all studied classes at unsampled locations, occurrence probability maps of single classes are needed..

Figures 11 and 12 show the occurrence probability maps of six classes, generated by MCG and SIS, respectively. These probability maps clearly show where and with how much uncertainty (or certainty) a class may occur. It is apparent that the occurrence probability maps of single classes generated by SIS are fuzzier than those generated by MCG. This means that given the same sample dataset the occurrence of a class at an unobserved location is more certain in simulated results by MCG than by SIS.

Figure 13 shows the difference map between the occurrence probability maps of six single classes generated by MCG and those by SIS. It can be seen that the classes generated by MCG are always convergent at several places with clear boundaries (see the blue areas in Fig. 13), but those generated by SIS are distributed in larger areas with moderate probabilities (including both the blue areas and red areas in Fig 13).

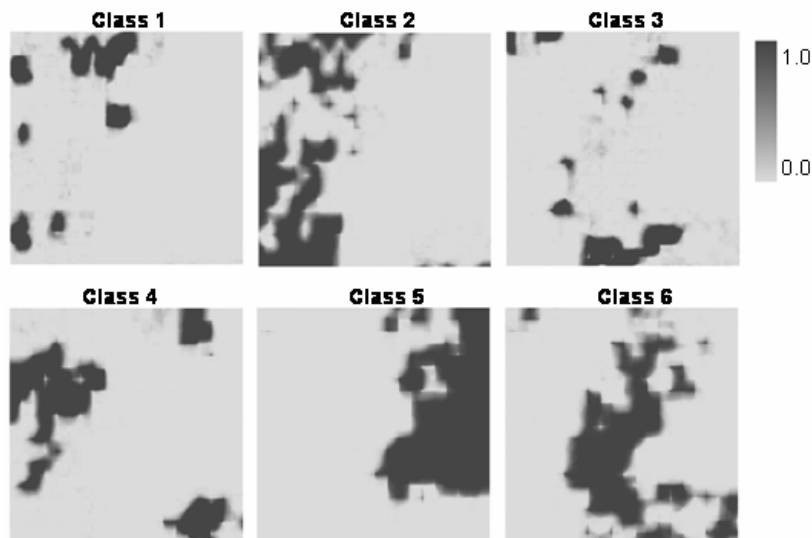


Figure 11. Occurrence probability maps of six single classes generated by MCG

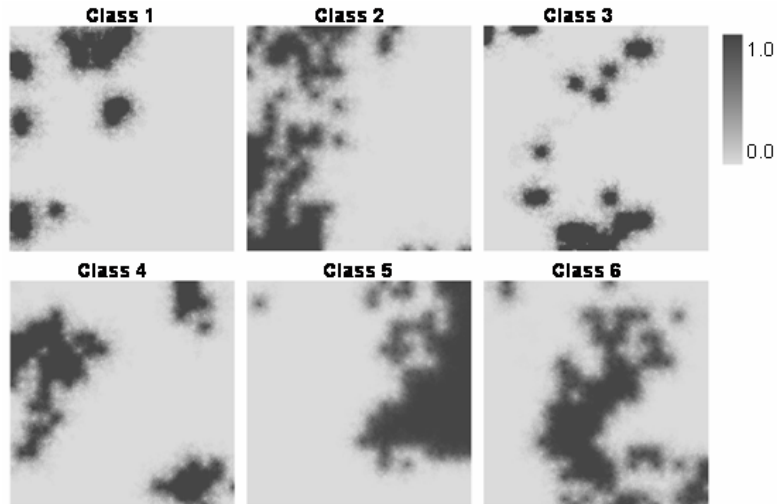


Figure 12. Occurrence probability maps of six single classes generated by SIS

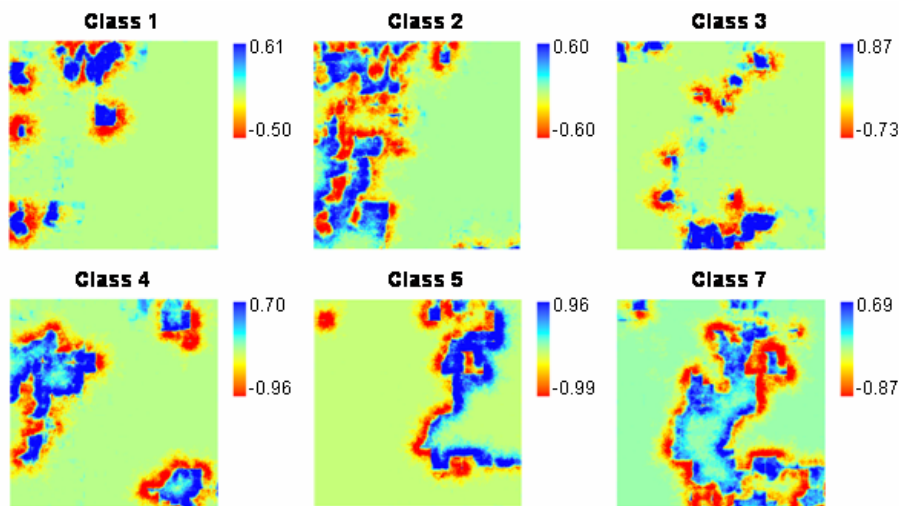


Figure 13. The difference map between occurrence probabilities of six classes generated by MCG and those by SIS (i.e., Difference = MCG data – SIS data)

4. Conclusions

The exact spatial uncertainty associated with a hand-delineated area-class map is never known, because human brains are generally too complex to quantify, let alone that an area-class map may be delineated by a team of experienced surveyors and map makers. However, it is clear that human brains seldom think questions linearly and they can incorporate complex knowledge from various sources into area-class mapping. Therefore, to exactly quantify the spatial uncertainty associated with a hand-delineated area-class map may be impossible. But it is also recognized that complex quantitative models may approach to the involved spatial uncertainty.

To effectively capture the spatial uncertainty of multinomial classes, important is that the approach used must be able to incorporate various spatial heterogeneity information conveyed by sample data and expert knowledge. Although as a practical technology indicator kriging geostatistics has been used to quantify spatial uncertainty of classes, it apparently deviates a lot from human minds in delineating area-class maps. MCG as an emerging nonlinear Markov

chain-based geostatistical approach is relatively closer to human minds in knowledge incorporation into area-class mapping.

Our simulated results using SIS and MCG demonstrated that MCG generates obviously less spatial uncertainty and higher PCC values than SIS does. This proved that interclass relationships and nonlinearity do play important roles in prediction, simulation, and spatial uncertainty assessment of multinomial classes. Because MCG is more mimic of human minds, we think that the spatial uncertainty assessed and visualized using MCG is closer to the real spatial uncertainty associated with human-delineated area-class maps. No doubt that human area-class mapping processes are very complex and spatial uncertainty arising in mapping is not limited to the spatial uncertainty caused by the limited number of samples. How to quantify the uncertainty caused by other sources, such as map generalization (e.g., omission of small polygons) and human mapping errors (e.g., wrong labeling), is still a challenging issue.

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