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SHORT COMMUNICATION

Some further clarification on Markov chain random fields and transiograms

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The Markov chain random field (MCRF) theory and the transiogram spatial measure were proposed several years ago. Basic sequential simulation algorithms based on simple MCRF models such as the Markov chain sequential simulation algorithm and the Markov chain sequential co-simulation algorithm have been developed and used in a series of application studies. However, misunderstanding of these two ideas and the geostatistical approach built on them arose recently among some researchers in geostatistics. The purpose of this article is to further clarify some issues related to these two ideas, so as to avoid further misunderstanding. For those issues already clarified, trivial, or obviously irrelevant, we do not talk about them here.

Keywords: Markov chain; transiogram; random field; geostatistics; categorical field

1. Introduction

The Markov chain random field (MCRF) theory (Li 2007a) and the transiogram spatial measure (Li 2007b) were proposed several years ago. Basic sequential simulation algorithms based on simple MCRF models such as the Markov chain sequential simulation (MCSS) algorithm and the Markov chain sequential co-simulation (Co-MCSS) algorithm have been developed and used in a series of application studies. The MCSS algorithm has proven to be superior to the indicator kriging-based sequential indicator simulation algorithm (Li and Zhang 2007). The Co-MCSS algorithm has shown to be a good method in improving the accuracy of remotely sensed land cover classification (Li and Zhang 2012a). However, misunderstanding of these two fundamental ideas and the geostatistical approach built on them arose recently among some researchers in geostatistics (Cao *et al.* 2011a, 2011b, 2012).

The MCRF theory was not sufficiently well described statistically to be a formal statistical theory in Li (2007a). To some extent, it is a plain idea for spatial modeling, but reasonably derived statistically. Because we have been working on environmental spatial modeling and geographical information technology, we did not make further efforts to have it widely recognized as a statistical theory in pure statistics or mathematics after it was published; on the contrary, we spent much energy on using the idea to application studies

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in different fields. However, this idea and the spatial statistical approach built on it have been recognized by statisticians; the core papers in proposing the MCRF approach with the transiogram spatial measure (e.g., Li 2007a, Li and Zhang 2007, 2008) were reviewed by well-known statisticians. Considering that some misunderstanding of the MCRF idea still exists and fresh misunderstandings may arise, we feel that we need make some further clarifications about the MCRF and transiogram ideas to the community.

In this article, we will try to clarify some issues related to these two ideas and the MCRF approach. The general purpose is to avoid further misunderstandings and arguments. For those issues already clarified, trivial, or obviously irrelevant, we will not discuss them here.

2. Further clarification of some related issues

2.1. On MCRFs

(1) The MCRF theory was not sufficiently described mathematically in our previous publications. In our opinion, the MCRF concept was a new idea for geostatistics or a primitive theory for spatial modeling purposes. That is why we have expressed that 'we welcome mathematicians or statisticians to have a rigorous treatment to the MCRF idea' (Li and Zhang 2012b). We said it was a theory because it was new, unique, statistically reasonable, and not a simple further deduction or adaption of an existing spatial statistical model. The MCRF theory does not involve complex mathematical deduction; such an idea is already enough for applied scientists in spatial modeling to develop useful specific operable methods. We said that MCRF models were theoretically sound, because (a) they avoided the exclusion of unwanted transitions and consequently corrected the small-class underestimation problem that occurred in the coupled Markov chain model proposed by Elfeki and Dekking (2001), (b) the solutions of MCRFs were reasonably derived using the Bayes' theorem, and (c) basic algorithms based on simple MCRF models worked well and proved to be superior to the widely used indicator kriging-based sequential indicator simulation algorithms. To our knowledge, the MCRF idea has advanced spatial modeling if viewed at least from the following aspects: (a) the previously proposed multidimensional Markov chain models in geosciences were not practical or did not condition on sample data (these do not include transition probability indicator kriging/cokriging, which were problematically described to be Markov chain models by some users and are also not nonlinear models); (b) Markov random field models proposed in statistics and image processing were traditionally implemented using iterative updating algorithms (these include Markov chain Monte Carlo methods); (c) Markov mesh models proposed in image analysis did not condition on sample data and usually used fixed consecutive paths (thus often leading to directional artifacts) (Li and Zhang 2008); and (d) the MCRF idea provided a typical nonlinear Bayesian inference geostatistical approach for conditional simulation of categorical fields on sparse sample data, which may generate simulated realizations in single sweeps. The conditional independence assumption was just used for implementation consideration without using multiple-point statistics. We did not simply apply the concept of Pickard random fields to general sparse cases. The property of Pickard random fields that given the value of the surrounded central pixel its four adjacent neighbors in cardinal directions are conditionally independent was reasonably extended to sparse data cases (Li 2007a), and this was used to support the neighborhood choice of using four nearest neighbors in four cardinal directions or four quadrants in MCRF algorithm design.

(2) The term 'random field' used in the MCRF approach is proper. It is widely known that a random field simply refers to a stochastic spatial process in one to multiple dimensions expressed by a random function. Although the term 'random field' was rarely used in

geostatistics, the term 'random function' in geostatistics means 'random field' (Chiles and Delfiner 1999). This is irrelevant to whether the property of a random field is fully known or not, and whether a random field has a stationary distribution or not. A random field does not need to have a spatially stationary distribution; there exist nonstationary random fields. Although a random field refers to a whole space of random variables (i.e., including all sites in a space), it is essentially defined by a generalized local (conditional or joint) probability distribution function on a neighborhood. In a sparse data situation, any local probability distribution is dependent on the local neighborhood structure. Given that a MCRF has the Markov property and also has the Markov chain characteristic, it is reasonable to call such a stochastic spatial process a *Markov chain random field*. However, MCRFs are different from classical MRF models, although the MRF concept in Besag (1974) covered various data situations: (a) classical MRF models were usually defined on lattice data with fixed neighborhoods (i.e., lattice-scheme neighborhoods), but MCRFs were defined on informed data (i.e., sample or simulated data) with a flexible neighborhood in a space in which data may be sparse irregular points; (b) classical MRFs are undirected, but MCRFs use directional interactions; (c) classical MRF models are not typical Bayesian inference models; however, MCRF models are typical Bayesian inference models with sequential updating on different nearest data; (d) classical MRF models were traditionally implemented using iterative updating algorithms (this implementation procedure may be regarded as Bayesian); on the contrary, MCRF models we used so far generated simulated realizations through single sweeps. A MCRF also can be defined on a lattice with a fixed neighborhood of adjacent sites but with directional interactions and Bayesian updating. However, that probably means it has to be implemented using the same way as classical MRF models were traditionally implemented, that is, using iterative updating algorithms from an initial image, which is obviously not our initial intention for an efficient geostatistical approach. In fact, MCRFs defined on lattice data are just special cases of the MCRFs defined in Li (2007a). In addition, MCRFs are also different from Markov mesh models (Abend *et al.* 1965) because the latter are always unilateral and were also defined on a lattice, thus being implemented using fixed consecutive paths. The first difference between MCRFs and classical MRFs is exactly the reason why the MCRF approach was called a geostatistical approach.

(3) The initial MCRF idea was for non-lattice point data of categorical spatial variables with a general setting of nearest neighbors. One can see this point from Li (2007a, pp. 325–327) and it was further emphasized in Li and Zhang (2012b). In our publications during the last several years, no matter whether it was articulated in one sentence or not, the MCRF definition was always that *a single spatial Markov chain moves or jumps in a space and decides its state at any uninformed location by interactions with its nearest neighbors in different directions*. This definition was intuitive but clearly stated the nature of MCRFs. Whether emphasizing 'including its last stay location' or not it does not matter, because this is implicit and one always can assume one of the nearest neighbors in a neighborhood to be the last stay location. In order to prove that the MCRF idea corrected the deficiencies of the coupled Markov chain idea it was first implemented on a rectangular lattice using fixed paths. Then, a random path simulation algorithm based on simplified MCRF models and transiograms was developed and used on sparse irregular point sample data. It is widely known that non-lattice spatial models can be used for lattice data or on a regular lattice (e.g., kriging models). We may consider implementing some multiple-point MCRF models in the future.

(4) We said that a MCRF is a special Markov chain or an extension of a one-dimensional Markov chain to multiple dimensions, because the MCRF idea was obtained in that effort

and a MCRF is indeed a single chain running in a space, but with local probability distribution updating on nearest data in different directions in a neighborhood. We said that MCRFs are special causal MRFs or might be regarded as an extension of Markov mesh random fields (or more generally MRFs) to geostatistics, because the latter were traditionally regarded in statistics as two-dimensional extensions of one-dimensional Markov chains; in fact, MCRFs do meet the general definition of MRFs (Cressie 1993, pp. 414–415). This also expressed our thought in the connection between the MCRF idea and the MRF theory, and our respect to Julian Besag and other pioneers who established the MRF theory, after all both the MRF theory and the Markov mesh theory gave us inspirations. However, the MCRF idea is a new spatial statistical idea different from classical MRF models. In order to use a single Markov chain to generate a random field, Li first had an idea of 'letting a Markov chain fly in a space like a Brownian motion but with interactions from nearest neighbors (samples or simulated data) in different directions at each uninformed location' and then gradually formulated the idea using the Bayes' theorem in a spatial context. There was not a direct mathematical deduction from a conventional existing Markov chain model, Markov mesh model, or MRF model to the MCRF solutions. Without the novel idea, there might not be a MCRF model and the resulting researches.

(5) The Bayes' factorization for spatial data in a Markov-type neighborhood was regarded as the *explicit full general solution* of MCRFs, as pointed out in Li and Zhang (2012b). This is exactly the advantage of MCRFs, because such a general solution can be simplified to whatever operable MCRF models and also can be expanded to hierarchical spatio-temporal MCRF models with data and knowledge from diverse sources. This full general solution for a local conditional distribution of MCRFs is expressed as

$$p[i_0(\mathbf{u}_0)|i_1(\mathbf{u}_1),\cdots,i_m(\mathbf{u}_m)] = A^{-1}p[i_m(\mathbf{u}_m)|i_0(\mathbf{u}_0),\cdots,i_{m-1}(\mathbf{u}_{m-1})] \cdots p[i_2(\mathbf{u}_2)|i_0(\mathbf{u}_0),i_1(\mathbf{u}_1)]p[i_0(\mathbf{u}_0)|i_1(\mathbf{u}_1)] \quad (1)$$

where A is the normalizing constant, $i_1(\mathbf{u}_1)$, $i_2(\mathbf{u}_2)$, ..., $i_m(\mathbf{u}_m)$ are the states of the nearest neighbors in different directions around the current uninformed location $\mathbf{u}_0$ being estimated, and $\mathbf{u}_1$ serves as the last stay location of the spatial Markov chain. If this factorization is for nonspatial data, it is irrelevant to spatial statistics; if it is only for lattice data, it is not much relevant to geostatistics; if it is for a rectangular lattice and has only two neighbors – the upper pixel and left pixel – it represents a correction of the simplest coupled Markov chain model (Elfeki and Dekking 2001, Li 2007a); however, if it is for non-lattice spatial data (e.g., spatially sparse sample data) and one can find some ways to implement it (usually its simplified forms), it can be a leap or revolution from Markov chains to geostatistics. That is exactly the initial idea of MCRFs (Li 2007a). This general solution clearly indicates the Bayesian inference characteristic of MCRF models, because it is in the form of

$$\text{posterior} \propto \text{likelihood}[i_m(\mathbf{u}_m)] \times \cdots \times \text{likelihood}[i_2(\mathbf{u}_2)] \times \text{prior} \quad (2)$$

where the prior is the transition probability function from the last stay location $\mathbf{u}_1$ to the current location $\mathbf{u}_0$ being estimated. The likelihood functions in this Bayes' factorization represent *simultaneous sequential Bayesian updating on different nearest data in a Markov-type neighborhood*. As a spatial Bayesian inference approach, MCRF models are always in the form or simplified forms of the Bayes' factorization. Although Bayes' factorization is not new and seems simple, what is new in the MCRF idea is *the Bayes' factorization for spatial point data in a neighborhood under the Markov property assumption and the single spatial Markov chain assumption*, which finally resulted in a new nonlinear spatial statistical approach for categorical data. Please note that the MCRF approach is mainly a multiple-point spatial statistics, but so far our implementations have been focused on using two-point statistics – the transiogram.

2.2. On transiograms

(1) The transiogram idea is not simply a name change of transition probability or a transition probability curve. Our initial purpose in proposing such a term and spatial measure was to find a way to estimate multiple-step transition probabilities and transition probability functions over the lag distance from sparse point sample data for Markov chain simulation. Later we found that it also could be an excellent independent two-point spatial measure for describing the spatial autocorrelations and interclass relationships of categories. Therefore, we further described the parameters and typical shapes of experimental transiograms and their physical meanings (Li 2006, 2007b). Both were inspired to a large extent by the variogram of classical geostatistics, and none of these was addressed by any study before ours. We are the first to estimate transiograms from sparse point sample data, the first to suggest practical transiogram joint modeling methods, and the first to use transiograms in Markov chain simulation. We recognized Schwarzacher (1969), Lou (1993, 1996), Carle and Fogg (1996, 1997), and Ritzi (2000) as pioneer studies in or related to transiograms and pointed out that Carle and Fogg (1996, 1997) were the most important pioneer studies on this topic (Li 2007b).

(2) The linear, spherical, exponential, and Gaussian models for autotransiograms provided in Li (2007b) were first suggested in Ritzi (2000), as cited in Li (2007b). Cross-transiogram models and hole-effect models were also provided in a table in Li (2007b). These were apparently also inspired by classical geostatistics. To the best of our knowledge, these models have been widely used as variogram models in kriging/indicator kriging for several decades (Goovaerts 1997). The purpose of suggesting these basic transiogram models was for users to use them singly or in nested models to fit the real shapes of experimental transiograms, which are reflections of the characteristics of real sample data. They have nothing to do with whether a categorical field is an indicator random field or truncated Gaussian random field. Whether a transiogram model is useful or not depends on whether it can fit the real shape of an experimental transiogram or not. As long as a transiogram model can meet the constraints of transition probabilities and it can be used in real application studies, it is generally valid. If transiogram models are used independently for the spatial variation description of categorical spatial variables (not simulation or interpolation), one even does not need to care whether a transiogram model can be accepted by any specific geostatistical model or not. Whether these transiogram models are valid to some specific random fields or geostatistical models with special assumptions is a topic for further study.

(3) Transition probabilities (or transiograms) can be quantitatively linked to indicator variograms by assuming that an indicator value is an occurrence probability of a category at a location (Carle and Fogg, 1996) using the following equation:

$$\gamma_{ij}(\mathbf{h}) = p_i\{p_{ij}(0) - [p_{ij}(\mathbf{h}) + p_{ij}(-\mathbf{h})]/2\} \tag{3}$$

where $\gamma_{ij}(\mathbf{h})$ represents the indicator variogram, $p_{ij}(\mathbf{h})$ and $p_{ij}(-\mathbf{h})$ represent the transiograms in opposite directions of the lag vector $\mathbf{h}$, and p_i represents the marginal probability of the category i. If categories i and j are the same, that is, for indicator autovariograms and autotransiograms, we have

$$\gamma_{ii}(\mathbf{h}) = p_i[1 - p_{ii}(\mathbf{h})] \tag{4}$$

However, cross-transiograms are normally asymmetric but indicator cross-variograms are always symmetric. Unidirectional cross-transiograms are normally irreversible, and thus cannot be derived from indicator cross-variograms or two-point joint probabilities. That is, indicator variograms can be defined by transiograms, but the converse is not true. This might be one of the major reasons why Carle and Fogg (1996) used transition probability to reformulate indicator kriging/cokriging, and thus made an interesting study. Apparently, it is not proper to simply use indicator variogram models to judge the general validity of transiogram models.

(4) The states or classes of a categorical field are represented by a series of labels (e.g., A, B, C, . . .), rather than indicator values (i.e., 0 and 1 values). A real categorical field does not need to be an indicator random field or truncated Gaussian random field and also does not need to have a spatially stationary probability distribution. While MCRF models have no other specific assumptions on sample data and spatial variables except for the Markov property (note that for transiogram estimation the intrinsic stationary assumption is needed, and for some simplified MCRF models the conditional independence assumption is needed), we have no reason to assume a real categorical field to be a specific theoretical random field (e.g., truncated Gaussian random field) and further apply constraints on transiogram models. If the shape of an experimental transiogram is too complex to be fitted by a basic transiogram model, one may use a nested model or composite model; if it still does not work, one may consider using other methods such as linear interpolation, as long as the experimental transiogram is reliable. If an experimental transiogram is not reliable (e.g., estimated from insufficient data), coarse model fitting of the general trend may be more practical. Li and Zhang (2010) and Li *et al.* (2012) provided some suggestions in transiogram modeling for the MCRF approach. It is possible that some transiogram models work for MCRF models but do not work for some other approaches such as indicator cokriging. However, what we have done is limited and was mainly for the MCRF approach; we did not test other approaches that might use the transiogram as their spatial measure. Further explorations are always necessary and open to the community. Other geostatistical methods that are based on other assumptions but use the transiogram may have specific requirements to transiogram models for those methods; this is a topic for further study. But that is irrelevant to the MCRF approach.

2.3. On conditional independence assumption

Our attitude to the conditional independence assumption is similar to Andre Journel's: his suggestion that this assumption should not be taken lightly and should be checked whenever possible (Journel 2002) was strongly emphasized in Li (2007a). That is also why we have been using the four nearest neighbors from four quadrants in the random-path MCSS algorithm while we proposed a very general approach, because this neighborhood design is the closest to being true in conditional independence of data. More complex MCRF simulation algorithms with or without the conditional independence assumption may be developed in the future. It turns out that Journel (2002) made a small mistake because the article stated that the data independence in the permanence of ratios was neither full nor conditional independence (Journel 2002, p. 584). That was why we said that the viewpoint of that 'the permanence of ratios is a general form of conditional independence' seemed arguable (Li and Zhang 2012b). But we do not think that the small error in Journel (2002) matters. There is no necessity to require a paper proposing an initial idea (i.e., the tau model, which was not implemented in this article) be perfect in every sentence.

If one is familiar with kriging, he/she may examine the implementation method of the tau model proposed by Cao *et al.* (2011a, pp. 1980–1981) to see its rationality: 'First the nearest neighbor x_1 of the target location x_0 is selected and we let $\tau_1 = 1$. Then, we assume the value $c(x_1)$ of this selected location x_1 is unknown and perform ordinary kriging (OK) to estimate it using the remaining neighbors as known data taking the OK weights as τ_n, $n > 1$.' We have no comment on their method. It is widely known that compromise through assumptions is often necessary in the practice of spatial statistics and the key is whether the compromise is rational and the method with the compromise is practical or not.

3. Conclusion

We have tried to clarify some issues related to the MCRF theory and the transiogram spatial measure, with the aim of avoiding further misunderstanding and arguments. The MCRF idea was proposed as an *approach* or *framework* for dealing with spatially sparse point sample data rather than as a specific model limited to lattice data. Its definition in Li (2007a) already stated this, although the development of random-path algorithms for dealing with irregular point sample data had to be delayed for a while. That was also the major reason why it was called a geostatistical approach. Our clarifications here are purely descriptive. To address the MCRF idea in detail statistically, a particular article is necessary.

One of the reasons that we called the MCRF approach 'Markov chain geostatistics' was to show our respect to Georges Matheron and other pioneers who founded the classical geostatistics, because we thought that geostatistics was a discipline or science rather than a set of existing techniques and thus should advance with the join of new ideas and approaches for similar purposes. This name followed those names such as 'indicator geostatistics', 'transition probability indicator geostatistics', 'multivariate geostatistics', 'modern geostatistics', 'model-based geostatistics', and 'multiple-point geostatistics', of which some are based on kriging, some are not, but all deal with sparse sample data. It is also apparent that the classical geostatistics inspired us a lot in developing the MCRF approach; for example, the transiogram is an analog to the indicator variogram. This name also showed our respect to Andrey Markov and other pioneers who founded the Markov chain theory because it indicated the Markov chain origin and nature of the MCRF approach. Probably, Markov chain geostatistics may cover more than the MCRF approach.

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