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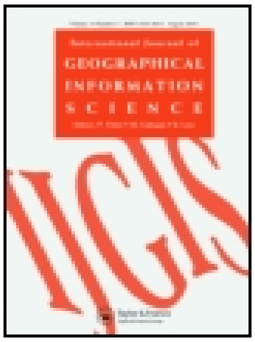

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RESEARCH ARTICLE

Examining the sensitivity of spatial scale in cellular automata Markov chain simulation of land use change

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ABSTRACT

Understanding the spatial scale sensitivity of cellular automata is crucial for improving the accuracy of land use change simulation. We propose a framework based on a response surface method to comprehensively explore spatial scale sensitivity of the cellular automata Markov chain (CA-Markov) model, and present a hybrid evaluation model for expressing simulation accuracy that merges the strengths of the Kappa coefficient and of Contagion index. Three Landsat-Thematic Mapper remote sensing images of Wuhan in 1987, 1996, and 2005 were used to extract land use information. The results demonstrate that the spatial scale sensitivity of the CA-Markov model resulting from individual components and their combinations are both worthy of attention. The utility of our proposed hybrid evaluation model and response surface method to investigate the sensitivity has proven to be more accurate than the single Kappa coefficient method and more efficient than traditional methods. The findings also show that the CA-Markov model is more sensitive to neighborhood size than to cell size or neighborhood type considering individual component effects. Particularly, the bilateral and trilateral interactions between neighborhood and cell size result in a more remarkable scale effect than that of a single cell size.

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Land use change simulation; cellular automata; Markov chain; spatial scale sensitivity; response surface method

1. Introduction

Cellular Automata (CA) has been recognized as one of the most promising methods to analyze complex systems, which is widely applied for simulating land use changes (White and Engelen 1997, Dietzel and Clarke 2006, Chen *et al*. 2017, Li *et al*. 2017). The changes resulting from the biophysical environment, socio-economic conditions, and human activities are often very complex (Valbuena *et al*. 2010, Wang *et al*. 2011a). Particularly, the complexity becomes more serious when these driving factors interact on each other (Wu 2002, Verburg and Veldkamp 2005). Numerous studies have suggested

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that CA models efficiently simulate these complex spatiotemporal processes and that they integrate well with raster-based remote sensing (RS) data (Torrens and O'Sullivan 2001, Li and Yeh 2002, Liu *et al*. 2010, Feng and Liu 2013). Therefore, research of land use change simulation using CA has been a hot topic in the field of geographic information science.

Because of the complexity of land use and cover change (Chen *et al*. 2014, van Vliet *et al*. 2016) and the hierarchy of CA models (Messina *et al*. 2008), CA-based land use change simulation results are sensitive to variations in their spatial scales (Li and Yeh 2001, Salap-Ayca *et al*. 2018), with different spatial scale combinations resulting in different outcomes (Moreno *et al*. 2009). This spatial scale sensitivity is usually generated from four components: cell size, neighborhood size, neighborhood type, and spatial extent (Menard and Marceau 2005). Among them, spatial extent is often associated with a given study case, such that it does not have a universal feature of spatial scale sensitivity during CA-based land use change simulation. Therefore, one should pay more attention to the other three components. As crucial parts of the CA model, their scale sensitivities have been extensively studied since 2000. For example, cell size is negatively correlated with simulation accuracy (Samat 2006), and Wang *et al*. (2011b) further explained the reasons behind the scale sensitivity in detail. Wu *et al*. (2012) concluded that a larger neighborhood size with planar neighborhood type contributed to a higher prediction accuracy, and Dahal and Chow (2015) used 30 neighborhood configurations to test the scale sensitivity and achieved an even more accurate simulation result. Both addressed individual components rather than the multiple component combinations of CA. Kocabas and Dragicevic (2006) used a comprehensive sensitivity analysis approach and concluded that the neighborhood configuration had a significant influence on the CA results apart from cell size. Pan *et al*. (2010) explored means in which multiple scale variations, including cell size and neighborhood configuration, as well as the spatial extent of the images, affected CA accuracy. Despite these significant contributions to the understanding of scale sensitivity of individual components in land use change simulation, no substantial research has yet been attempted to investigate how the sensitivity relates to the interactions of different scale combinations. After all, the existing interactions within the CA model at different scale combinations may seriously affect the simulation accuracy if there are no measures implemented to reduce the scale sensitivity.

The transition rule is another core part of CA theory (Liu *et al*. 2008). Many transition rules have been formulated based on various internal laws of land use conversion, such as Markov chain (Kamusoko *et al*. 2009), neural network (Li and Yeh 2002), genetic algorithm (Shan *et al*. 2008), ant colony optimization (Liu *et al*. 2008), and data mining (Li and Yeh 2004). Among them, the CA-Markov model has been increasingly regarded as a robust approach for simulating land use changes (Kamusoko *et al*. 2009). One important advantage of CA-Markov is simultaneously predicting the trajectory of land use change among various categorical states (Pontius and Malanson 2005, Feng 2017) and simulating spatio-temporal dynamic changes (Li *et al*. 2016) to improve the simulation accuracy as much as possible, although it only models land use changes using a constant time step (Jenerette and Wu 2001). Guan *et al*. (2011) forecasted the future land use changes in Saga during the period 2015–2042 integrating the CA-Markov model with natural and socio-economic data. Halmy *et al*. (2015) used the CA-Markov integrated approach to predict land use change and project changes by extrapolating current trends in the northwestern desert of Egypt. Hyandye and Martz (2017) simulated Usangu catchment's land use change for 2020 using CA-Markov analysis to investigate the effect of land use change on water balance in the catchment. As for the scale sensitivity of the CA-Markov model for land use change simulation, Wu *et al*. (2013b) used the orthogonal test method to examine the interaction at different scale combinations. Nevertheless, using this methodology to identify the optimal scale combination of the CA model among a severely limited range, in general, may produce misleading results, or even miss the optimal scale combination. Fortunately, the response surface method (RSM), which merges the strengths of the steepest ascent method with those of the central composite design, has significantly improved our ability to determine the optimal scale combination (Joyce and Leung 2013). In contrast, RSM is not only more efficient in computational tasks (Zhang and Liu 2015) but is also more explicit in interaction analyses (Tran *et al*. 2016) than the orthogonal test method could be. These characteristics allow one to fully consider more potential combinations in the CA model to better understand the scale sensitivity of CA-Markov in land use change simulation. Notably, the operational objects of any transition rule remain the cell and neighborhood during the whole CA simulation. This means that the spatial scale sensitivity of the transition rule essentially originates from that of the cell and neighborhood.

The objective of this study was to use the RSM to explore the scale sensitivity of the CA-Markov model in land use change simulation. In particular, we investigated whether or not the components or their combinations interact at different spatial scales, and then determined how they affect the simulation accuracy. This will allow governmental organizations to identify the optimal scale combination for predicting land use change to achieve better decision making for urban development planning.

2. Study area and data

2.1. *Study area and data*

Wuhan, similar to other Chinese cities such as Beijing, Shanghai, and Shenzhen, has undergone rapid land use change over the last three decades (Wu *et al*. 2014). Between the middle 1980s and early 2010s, Wuhan underwent two important development stages. One was the rapid urban construction because of the support of the practice market economy from the Chinese government, and the other was urban economic recovery because of the implementation of a series of key transportation projects. Given that a large area of arable land has been converted to urban land use in Wuhan, it provides a good case in which to test the scale sensitivity of CA. This area is situated in the eastern part of Hubei Province, centered at 113°41′115°05′E longitude and 29°58′-31°22N′ latitude as shown in Figure 1. The administrative area of Wuhan covers approximately 8549 km^2, approximately 10.4% of which is the central district, while the remaining 89.6% consists of rural districts.

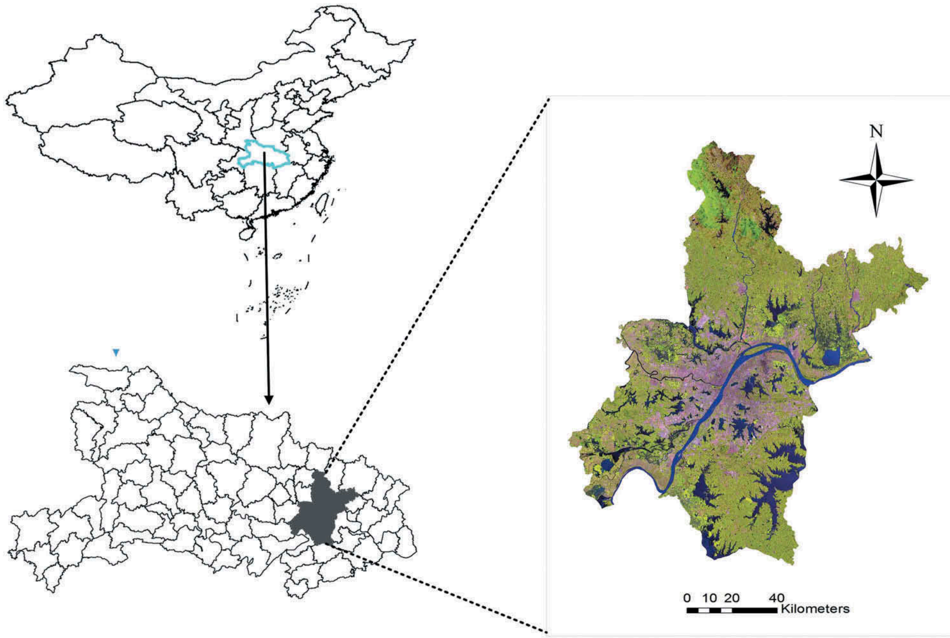

Figure 1. Location of the study area, Wuhan, China.

2.2. *Image and image pre-processing*

Three Landsat-Thematic Mapper (TM) remote sensing images of Wuhan (provided by the Computer Network Information Center) in 1987, 1996, and 2005 were used to map the land use at a 30-m resolution. These images were projected to the Universal Transverse Mercator (UTM) system (datum WGS84 and UTM Zone N49) and resampled using the maximum likelihood method. After ENVI@RSI 5.1 was used to pre-process these data, they were then converted into a TIFF format in ArcGIS@ESRI 10.2. To facilitate the computation and model operation, the land use types in the original images were finally reclassified into the five shown in Figure 2: water, construction land, forest, arable land, and unused land.

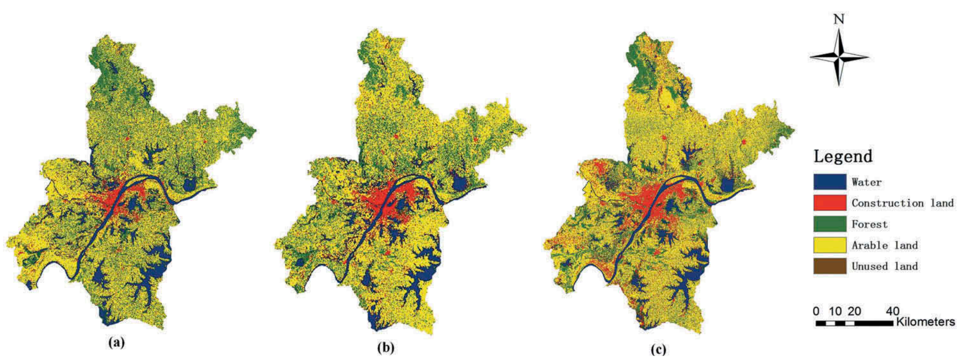

Figure 2. Three land use classification maps of Wuhan: (a) 1987, (b) 1996, and (c) 2005.

3. Methods

3.1. *Markov chain analysis*

The Markov chain analysis is a stochastic process model that makes use of the transition probability to simulate land use change between two land use types (Mondal and Southworth 2010). The transition probability (P_{ij}) is determined by the number of pixels that change from land use type i in time t to land use type j in time $t+1$ as follows:

$$P_{ij} = n_{ij}/n_i \tag{1}$$

$$\sum_{j=1}^{m} P_{ij} = 1 \tag{2}$$

where$n_i$is the total number of pixels of type i, n_{ij} is the number of pixels that transform from type i to type j, and m is the number of land use types. The transition probability matrix Pwhich is composed of P_{ij}, is used to analyze the change from time t to $t+1$ as follows:

$$V_{t+1} = P \times V_t \tag{3}$$

where $V_{t+1}$and V_t are two consecutive state vectors at time$t+1$and t, respectively.

3.2. *RSM for spatial scale sensitivity*

The scale sensitivity of CA-Markov is mainly in relation to three factors: cell size, neighborhood size, and neighborhood type. We used the RSM to explore their effects on simulation accuracy. There are two key steps, namely the experimental design of the steepest ascent method and the central composite design.

3.2.1. *Experimental design of the steepest ascent method*

To minimize the scope of the experimental design and approach the optimal scale as rapidly as possible, the steepest ascent method was used to aggregate the variations in the aforementioned three factors from a coarse scale to fine scale. The steepest ascent method can take advantage of the potential information involved in the optimal scale to describe a particular response, which is expressed by an object function value. This is helpful in that it allows one to obtain reasonable experimental combinations, rather than subjectively selecting or guessing as is typical. This procedure does not stop until the combination closest to the optimal scale is fully identified.

The neighborhood types used in this study, Moore and Von Neumann, are the most commonly applied in the two-dimensional raster-based CA-Markov method (Balzter *et al*. 1998, Wu *et al*. 2012). Because of the negative correlation between the simulation accuracy and the size of the cell and neighborhood, their sizes are initially set at a coarse scale and progress to a fine scale. These scales and their combinations are sufficient to explore the potential information regarding how the scale sensitivity behaves during land use change simulation, such that one can determine finite center points from numerous initial points on behalf of different scales.

3.2.2. *Central composite design*

Central composite design (CCD) was applied to optimize the particular response affected by the aforementioned predetermined independent variables. The extraction variables included cell size (X_1), neighborhood size (X_2) and neighborhood type (X_3). Both X_1 and X_2 were coded at five levels (−1.41, −1, 0, 1, and 1.41) representing the lowest, lower, middle, higher, and highest values, while X_3 was coded at its two levels (−1 and 1) that represent the Moore and Von Neumann neighborhoods, respectively. These coded values were generated in the software of Design-Expert@ Stat-Ease 8.0.6. During the central composite design process, the actual values corresponding to these coded values were provided with consideration of the data situation. Among them, the maximum, middle, and minimum actual values of cell and neighborhood sizes, which correspond to these coded values at three levels (−1.41, 0, and 1.41), were directly derived from the experimental results of the steepest ascent method. Other actual values were calculated using the ratio of the coded values and using the determined cell size as well as the neighborhood size. The calculated actual values of cell size needed to be rounded to the nearest integral multiple of the raw pixel resolution to provide convenience during the RS image processing, and the calculated actual values of neighborhood size needed to be rounded to the nearest odd number to meet the operating requirement of the CA-Markov model. Then, we used the central composite design, which integrates the aforementioned different spatial scale combinations with the corresponding simulation accuracy evaluation indices, to build a series of trials to fully explore the spatial scale sensitivity of the CA-Markov land use change simulation. The number of trials was determined by the number of variables, and the scheme of the experiment was designed according to the actual values of these variables.

To quantify the unilateral, bilateral, and trilateral effects of cell size (X_1), neighborhood size (X_2), and neighborhood type (X_3) on the CA-Markov land use change simulation, a third-order equation was employed to fit these three variables using the least squares regression method as follows:

$$Y = a_0 + \sum_{\substack{i,j=0 \\ i+j \leq 1}}^{1} b_{ij}x_1^i x_2^j x_3^{1-i-j} + \sum_{\substack{i,j=0 \\ i+j \leq 2}}^{2} c_{ij}x_1^i x_2^j x_3^{2-i-j} + \sum_{\substack{i,j=0 \\ i+j \leq 3}}^{3} d_{ij}x_1^i x_2^j x_3^{3-i-j} \tag{4}$$

where Y is the response value; x_1,x_2, andx_3 are the predetermined independent variables; a_0 is the intercept; and b_{ij},c_{ij}, and d_{ij} are the regression coefficients for the linear, quadratic and cubic components, respectively. In this study, the analysis of variance (ANOVA) test was employed to determine the statistical significance of these regression coefficients, and the model adequacy of the third-order equation to the responses was estimated by the coefficient of determination (R^2). The statistical significance of the terms was evaluated by calculating the F value at the level of $p < 0.05$. We replicated each experiment and recorded the hybrid evaluation values as the response. Once the fitted regression equations and the ANOVA test were completed, the three-dimensional (3D) response surface and contour plots were generated using the Design-Expert@ Stat-Ease 8.0.6 software. They were drawn by running any two variables while maintaining the others constant.

3.3. *Hybrid evaluation model of simulation accuracy*

The sensitivity evaluation of CA is often quantified by the accuracy of land use change simulation. Previous studies have shown that the Kappa coefficient is the most commonly used method to evaluate the accuracy of land use change CA-based simulation (Kocabas and Dragicevic 2006, Fuglsang *et al*. 2013, Al-Sharif and Pradhan 2014). It is a statistical measure of the agreement between the simulated land use map and the classified land use map (van Vliet *et al*. 2011), but fails to describe the detailed spatial distribution of the CA-based simulation error (Samat 2006). In terms of the spatial scale-induced agreement, it is necessary to provide both a statistical solution to the simulation accuracy of the CA-Markov model at the total level and a spatial solution for its error distribution at the local level. To describe the detailed spatial error distribution, the Contagion index from the landscape, which can quantitatively measure both patch type interspersion and patch dispersion at the landscape level (McGarigal 2015), was introduced. During the evaluation of land use change simulation accuracy, we used the Contagion index to quantify the interspersion between error patches and non-error patches, and the spatial distribution of a certain patch type. Therefore, we built a hybrid model to express the spatial scale sensitivity of the CA-Markov model for land use change simulation, which integrated the Kappa coefficient with the Contagion index as follows:

$$H = W_k P_k + W_c (A - P_c) \tag{5}$$

where H is the value of the hybrid evaluation. It represents the land use change simulation accuracy of CA-Markov at a certain scale combination, which is the observational value corresponding to response value Y in Equation (4). $P_k$and$P_c$are the Kappa coefficient and the Contagion index, respectively, that are standardized using the Z-score method. $P_k$is positively related to simulation accuracy, while$P_c$is negatively related. $A$is the maximum interval distance of the post Z-score standardization to make the hybrid evaluation value greater than 0. $W_k$and $W_c$are the weights of the Kappa coefficient and contagion index, respectively.

The Kappa coefficient was calculated in the CROSSTAB module of IDRISI Andes@ Clark University Laboratory 15.0 by comparing the simulated land use map to the classified land use map. Meanwhile, we also obtained a cross-classification image that contains the information regarding the simulation error distribution and then used for calculating the contagion index as follows (McGarigal 2015):

$$CONTAG = \left\{ \sum_{i=1}^{m} \sum_{k=1}^{m} \left[\left(P_i - e_{ik} / \sum_{k=1}^{m} e_{ik} \right) \ln \left(P_i - e_{ik} / \sum_{k=1}^{m} e_{ik} \right) \right] / 2 \ln m + 1 \right\} \times 100 \tag{6}$$

where CONTAG is the Contagion index value; P_i is the proportion of the landscape occupied by land use patch type$i$, which was classified during the land use change simulation experiment; $e_{ik}$is the number of adjacencies between the pixels of land use patch types$i$and$k$based on the double-count method; and m is the number of land use patch types that are present in the landscape. After the cross-classification image was reclassified as an error patch or non-error patch in ArcGIS@ ESRI 10.2, the contagion index was calculated using Fragstats@ UMass Landscape Ecology Lab 4.2. The contagion index approaches 0 when the spatial distribution error is maximally disaggregated. Conversely, it approaches 100 when the error is maximally aggregated. For accurate simulation of land use change, the uniformity of the spatial distribution error is very important. A lower contagion index means the spatial error is maximally disaggregated and there is equal distribution. That is to say, the contagion index is negatively related to simulation accuracy.

Determining the weights of the Kappa coefficient and contagion index is also a key step in the hybrid evaluation model of spatial scale sensitivity. Here, $W_k$and $W_c$were determined using the entropy method, which is an objective method of weight determination. This method determines weights according to the information provided by the Kappa coefficient and contagion index in quantifying the scale sensitivity of the CA-Markov model. The weights were calculated using MATLAB@ MathWorks R2012a, and a detailed explanation of entropy weight has been provided by (Zou *et al*. 2006).

3.4. *Flow of exploring the spatial scale sensitivity of the CA-Markov model*

The framework used to explore the spatial scale sensitivity of the CA-Markov model for land use change simulation is shown in Figure 3. In order to avoid the subjective choice of transition rules, we used the collection of transition suitability maps without any other factors, obtained by constant prediction based on a transition probability matrix. In the experimental design of the steepest ascent method, the cell and neighborhood sizes were set as 330 m, 270 m, 210 m, 150 m, 90 m, and 30 m and 23, 19, 15, 11, 7, and 3, respectively, and the neighborhood types were Von Neumann and Moore neighborhoods. After simulating the land use changes using the CA-Markov model with these different scale combinations, the potential center points at the optimal scale were chosen by comparing the hybrid evaluation values. Then, the experimental scheme of the central composite, employing these center points, was designed using Design-Expert@ Stat-Ease 8.0.6. Likewise, the trials of different scale combinations in the central composite design were performed using the IDRISI software. Finally, we obtained the optimal scale combination and then discussed the individual component effect as well as component combination interaction effect via a comprehensive analysis using the ANOVA test and contour and 3D response surface plots.

4. Results

4.1. *CA-Markov simulation results of land use change*

The nature of land use change from 1987 to 1996 can be quantified by the transition trend as depicted from the Markov transition probability matrices. According to Equation (1), we used both classification land use maps for 1987 and 1996 to calculate a series of Markov transition probability matrices at different cell sizes. During the experiments using the steepest ascent method and central composite design, 6 and 26 transition probability matrices were obtained, respectively. Because the transition probability matrix is related to cell size rather than neighborhood size and neighborhood type in the CA-Markov model, there were six transition probability matrices from the experiment using the steepest ascent method. For example, the transition

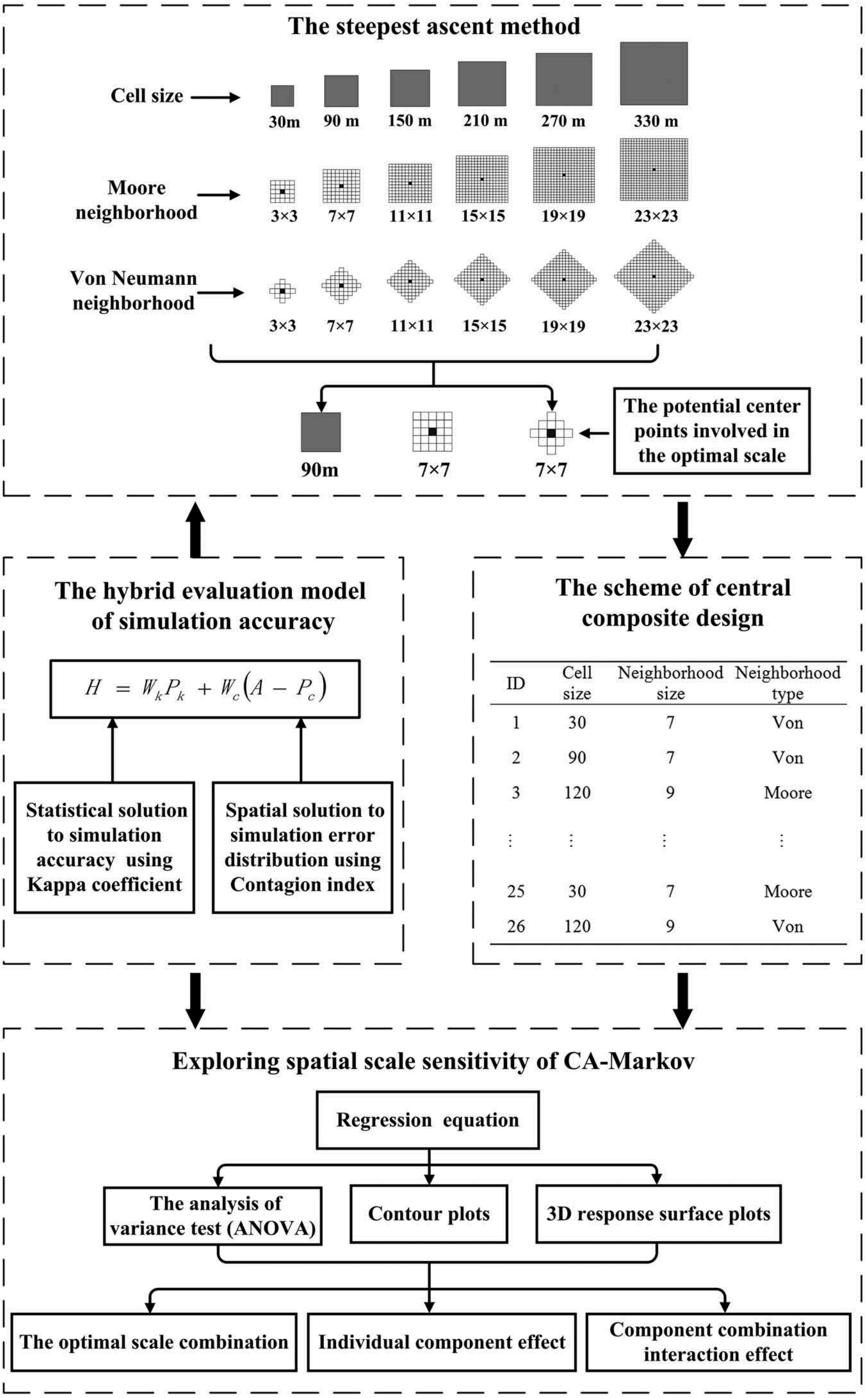

Figure 3. Flowchart for exploring the spatial scale sensitivity of the CA-Markov model using the RSM.

probability matrix at a cell size of 30 m during the experiment of the steepest ascent method is provided in Table 1. It shows that the construction land yields the highest transition probability (0.6385), followed by arable land (0.6030), water (0.5712), forest (0.3208), and unused land (0.0415) in a diagonal line. This result indicates that construction land, arable land, and water mainly persisted from 1987 to 1996, with transition probabilities greater than 0.5. Both forest and unused land are different from those three land use types, with low probability of persistence during this stage. Notably, apart from arable land, the lowest probability of undergoing no change was that of forest, which was just 0.3208, while the transition probability from forest to arable land reached 0.5604. Similarly, the transition probability from unused land to arable land was 0.6112. These results suggest that substantial amounts of forest and unused land were converted into arable land from 1987 to 1996. If we consider the family-contract responsibility system in 1981, which is regarded as a significant breakthrough and innovation in rural land property rights in China (Wu *et al*. 2013a), the transition probability shown in Table 1 seems reasonable.

Figure 4 shows that 12 groups of CA-Markov land use simulation results for 2005 were obtained using the aforementioned six transition probability matrices, which were used during the experiment of the steepest ascent method. These simulation maps were generated from different scale combinations, in which the cell sizes ranged from 30 m to 330 m and neighborhood size from 3 to 23, under the two different neighborhood types, Moore and Von Neumann. Figure 4(a,b) show that the simulation results with a cell size of 30 m and neighborhood size of 3 are both fine, while Figure 4(k,l) show that

Table 1. Transition probability matrix from 1987 to 1996 (30-m cell size, 3-neighborhood size).

	Water	Construction land	Forest	Arable land	Unused land
Water	0.5712	0.0820	0.1455	0.1942	0.0071
Construction land	0.1074	0.6385	0.1360	0.1056	0.0124
Forest	0.0723	0.0418	0.3208	0.5604	0.0047
Arable land	0.0440	0.0797	0.2610	0.6030	0.0124
Unused land	0.1010	0.1682	0.0780	0.6112	0.0415

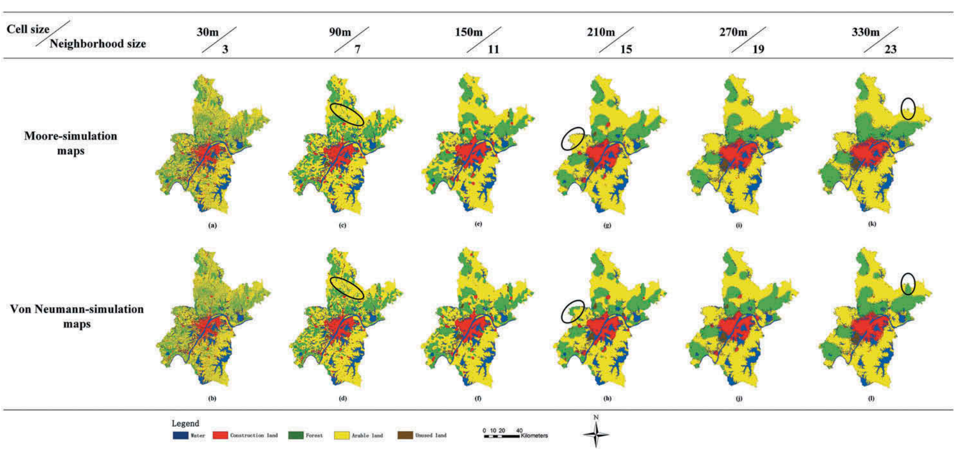

Figure 4. Results of the land use change simulation at six spatial scale combinations from the experiment using the steepest ascent method in 2005.

the simulation results with a cell size of 330 m and neighborhood size of 23 are both coarse. This indicates that the CA-Markov simulation accuracy continuously decreases during the upscaling process of cell size and neighborhood size. Notably, the apparent difference between Figure 4(k,l), which has been marked using two black ellipses, shows that the simulation result is forest using the Von Neumann neighborhood type while it is arable land using the Moore neighborhood type when the cell size and neighborhood size are both the same. The same difference exists at a scale of a 90-m-sized cell as shown in Figure 4(c,d) and the scale of a 210-m-sized cell as shown in Figure 4(g,h). This illustrates that the scale effect induced by cell and neighborhood size and neighborhood type has an obvious influence on the simulation accuracy of the CA-Markov model for land use change.

4.2. *Experimental design results of the steepest ascent method*

The Kappa coefficient calculated by comparing the classification land use maps for 2005 to the 12 groups of CA-Markov land use simulation results for the experiment using the steepest ascent method is provided in Table 2. It shows that the Kappa coefficient ranges from 0.7062 to 0.6719. Although the Kappa coefficient decreases during the upscaling process of cell and neighborhood size, the differences are not very great. In fact, these slight differences in the Kappa coefficient shown in Table 2 are inconsistent with the great differences in the CA-Markov land use simulation results shown in Figure 4. In other words, the simulation accuracies under different scale combinations are not statistically different. The reason for this is that Kappa coefficient is just a statistical measure of the agreement and thus fails to describe the detailed spatial distribution of the CA-based simulation error. This confirms that the Kappa coefficient is not sufficient to evaluate the accuracy of land use change simulation. This is why we developed a hybrid evaluation model to improve upon the Kappa coefficient evaluation system.

According to Equation (6), the contagion index that quantifies the dispersion of simulation error is provided in Table 2. It shows that the contagion index has a clear variation, ranging from 15.0459 to 4.8176. This suggests that the simulation error distribution maximally aggregates at a scale of a 30-m cell and 3 neighborhoods, while it maximally disaggregates at a scale of a 330-m cell and 23 neighborhoods using the Moore neighborhood type. This result indicates that the error of the CA-Markov land use simulation result gradually disaggregates as the cell size and neighborhood size upscale. This demonstrates that it is feasible to use the contagion index to

Table 2. Experimental design results of the steepest ascent method.

			Kappa coefficient		Contagion index		H_M	H_V
ID	Cell size	Neighborhood size	Moore*	Von*	Moore	Von	Moore	Von
1	30	3	0.7062	0.7058	15.0459	13.5908	1.3081	1.1055
2	90	7	0.6959	0.6982	8.7081	8.6070	1.3237	1.1460
3	150	11	0.6885	0.6918	7.0571	7.0980	1.0617	0.9270
4	210	15	0.6821	0.6844	6.0261	6.1454	0.7977	0.5992
5	270	19	0.6735	0.6785	5.2311	5.2959	0.3873	0.3463
6	330	23	0.6719	0.6747	4.8176	4.8744	0.3359	0.1716

*Moore: Moore neighborhood type
*Von: Von Neumann neighborhood type.

evaluate the simulation error spatial distribution of the CA-Markov model for land use change.

Twelve hybrid evaluation values of simulation accuracy at different scales, derived from the Kappa coefficient and contagion index using Equation (5), are shown in Table 2. The table shows that the hybrid evaluation values can be sorted in descending order as 1.3237, 1.3081, 1.0617, 0.7977, 0.3873, and 0.3359 using the Moore neighborhood type, and 1.1460, 1.1055, 0.9270, 0.5992, 0.3463, and 0.1716 using the Von Neumann neighborhood type. For the Moore neighborhood type, the hybrid evaluation value reaches a maximum (1.3237) at a cell size of 90 m and neighborhood size of 7 and a minimum (0.3359) at a cell size of 330 m and neighborhood size of 23. When the cell size ranges from 30 m to 150 m and the neighborhood size ranges from 3 to 11, these hybrid evaluation values of different scale combinations are remarkably higher than those within the 210 m to 330 m cell size and 15 to 23 neighborhood size. Therefore, the potential center points in the optimal scale lie within a cell size of from 30 m to 150 m and a neighborhood size of from 3 to 11. The same tendency occurs for the Von Neumann neighborhood type.

4.3. *Optimal scale combination results of the CA-Markov model in central composite design*

The actual values of cell size and neighborhood size at five different levels in the central composite design are provided in Table 3. They were determined by potential center points within the cell size range of from 30 m to 150 m and the neighborhood size range of from 3 to 11. For these actual values of cell size, 30, 90, and 150 were derived from the aforementioned experiment results using the steepest ascent method, while 60 and 120 were approximately calculated using the ratio of 1.41 to 60, where 1.41 is the difference from 0 to ±1.41 and 60 is the difference from 90 to 30 or 90 to 150. Similarly, the actual values of the neighborhood size at five different levels were calculated. In addition, the neighborhood type coded at two levels is also shown in Table 3, which includes the Moore and Von Neumann neighborhood types.

The trial scheme of the central composite design was designed using the aforementioned neighborhood type and actual values of cell size and neighborhood size. The trial number determined by these three spatial scale sensitivity components was 26 (Table 4). There were 13 trials under each neighborhood type. Five of the 26 trials were repeated at a cell size of 90 m and a neighborhood size of 7 using either neighborhood type, which were automatically generated from the Design-Expert software, so as to validate whether a certain distinct difference in the hybrid evaluation values existed at the potential optimal scale combination. For the Moore neighborhood type, its hybrid evaluation value reached a maximum of 2.4857 and a minimum of 0.3964. For the

Table 3. Cell size, neighborhood size, and neighborhood type at different levels in the central composite design.

Coded values	−1.41	−1	0	1	1.41
Cell size	30	60	90	120	150
Neighborhood size	3	5	7	9	11
Neighborhood type	N/A	Moore	N/A	Von	N/A

Table 4. Results of the spatial scale combination and its accuracy evaluation on CA-Markov land use change simulation results from 26 trials in the central composite design.

ID	Cell size	Neighborhood size	Neighborhood type	Kappa coefficient	Contagion index	H
1	30	7	Von	0.7040	16.3136	1.5099
2	90	7	Von	0.6982	8.6070	1.6392
3	120	9	Moore	0.6905	7.7196	0.3964
4	120	5	Moore	0.6969	7.6471	1.5520
5	90	11	Von	0.6948	8.7179	1.0143
6	90	3	Von	0.7034	7.1568	2.7888
7	90	7	Moore	0.6959	8.7081	1.2125
8	60	9	Moore	0.6965	10.7021	1.0180
9	90	7	Von	0.6982	8.6070	1.6392
10	150	7	Moore	0.6923	7.0708	0.8165
11	60	5	Moore	0.7010	10.4910	1.8548
12	90	7	Moore	0.6959	8.7081	1.2125
13	90	7	Moore	0.6959	8.7081	1.2125
14	90	7	Von	0.6982	8.6070	1.6392
15	90	7	Moore	0.6959	8.7081	1.2125
16	60	9	Von	0.6990	10.5929	1.4816
17	90	7	Moore	0.6959	8.7081	1.2125
18	90	11	Moore	0.6920	8.7196	0.5133
19	60	5	Von	0.7027	10.0575	2.2244
20	150	7	Von	0.6952	6.9787	1.3491
21	120	5	Von	0.6993	7.3936	2.0196
22	90	3	Moore	0.7024	7.9775	2.4857
23	90	7	Von	0.6982	8.6070	1.6392
24	90	7	Von	0.6982	8.6070	1.6392
25	30	7	Moore	0.7026	16.6857	1.2032
26	120	9	Von	0.6940	7.6917	1.0266

Von Neumann neighborhood type, its hybrid evaluation value reached a maximum of 2.7888 and a minimum of 1.0143. Both had the maximum hybrid evaluation value at a cell size of 90 m and neighborhood size of 3. This indicates that the optimal scale combination of the CA-Markov model for land use change simulation should be near a 90-m cell size and 3 neighborhoods using Von Neumann neighborhood type. The simulation results of land use change at this spatial scale combination are shown in Figure 5. In addition, this suggests that both the potential center points of the central composite design and the optimal scale combination of the CA-Markov model lie within the scale range from the steepest ascent method. This validates that it is reasonable to use the steepest ascent method in advance of the central composite design.

4.4. *Results of spatial scale effects of the CA-Markov model on land use change simulation*

Based on 26 trials in the central composite design, the simulation accuracy variation in land use change is provided using contour and 3D surfaces (Figure 6). The red, green, and blue represent better, good, and poor simulation results for land use change, respectively. These results show that a better simulation result of land use change occurred at a scale range of from the 30 to 90 m for cell size and from 3 to 5 for neighborhood size under both neighborhood types. Figure 6(a) shows that the blue areas expanded the most, followed by the green and red areas using the Moore neighborhood type, while it ranked in descending order as green areas, red areas, and blue areas using the Von Neumann neighborhood type as shown in Figure 6(b). It is

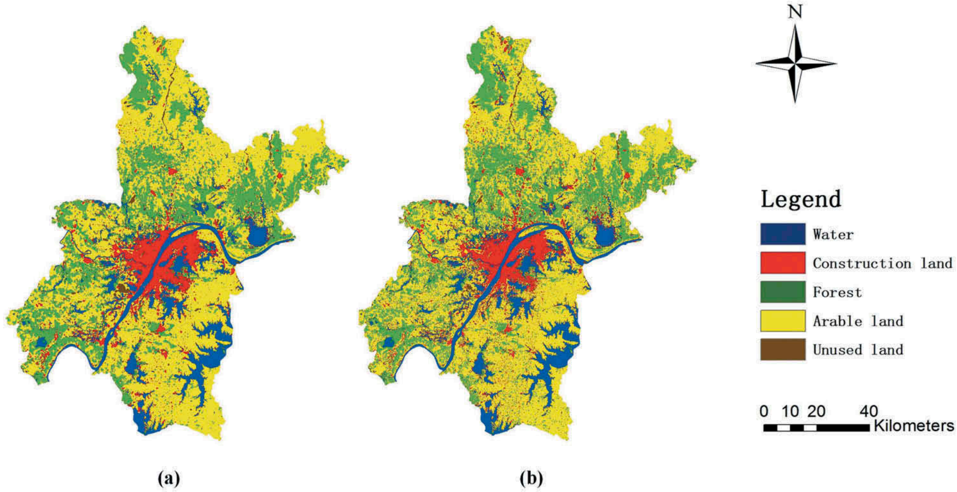

Figure 5. Simulation results of land use change simulation at a 90-m cell size and 3 neighborhoods: (a) Moore neighborhood type (b) Von neighborhood type.

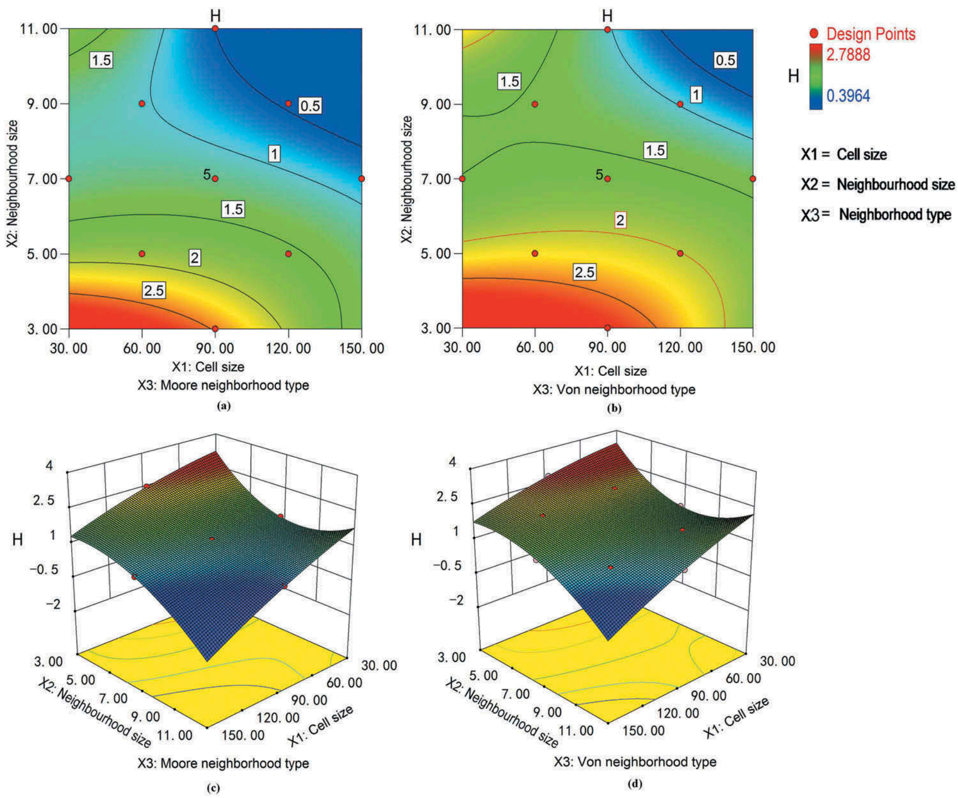

Figure 6. Contour and 3D surfaces for simulation accuracy variation for land use change.

obvious that there are larger red areas using the Von Neumann neighborhood type than using the Moore neighborhood type. This suggests that the scale range of better simulation accuracy using the Von Neumann neighborhood type is broader than that of the Moore neighborhood type. This indicates that the CA-Markov model is more sensitive to spatial scale change using the Von Neumann neighborhood type than using the Moore neighborhood type. In addition, the 3D surfaces of the change trends from these hybrid evaluation values are provided in Figure 6(c,d).

5. Discussion

5.1. *Complexity of spatial scale sensitivity in the CA-Markov model*

Many studies have explored the scale sensitivity of individual components of the CA-Markov model (including cell size and neighborhood size and type) rather than that of their combinations. To further identify whether the components or their combinations affect the simulation results at different scales, we performed ANOVA for 26 trials from the central composite design. Cell size, neighborhood size, and neighborhood type have highly significant ($p < 0.0001$) unilateral (X_1, X_2, andX_3) effects on simulation accuracy and consequently show scale sensitivity (Table 5). This has been demonstrated by previous studies (Kocabas and Dragicevic 2006, Samat 2006, Altartouri *et al*. 2015). Notably, we also found that the quadratic terms (X_1^2andX_2^2) have significant ($p < 0.0001$) effects, suggesting that they are both characterized by scale sensitivity. In addition, their bilateral interaction (X_1X_2, X_1X_3, andX_2X_3) and trilateral interaction ($X_1X_2^2$) also have high significance ($p < 0.0001$) and show the phenomenon of scale sensitivity. It is clear that these different component combinations result in considerable effects on the accuracy of land use change simulation. This demonstrates that there are strong component interactions in the CA-Markov model at different spatial scales. The findings show that the CA-Markov model is sensitive to spatial scale change from not only individual components but also from their combinations. On the basis of the aforementioned analysis, one should consider the complexity of spatial scale sensitivity in the CA-Markov model if intending to improve its accuracy of land use change simulation.

When exploring the complexity of spatial scale sensitivity in the CA-Markov model, efficiency is another important factor that one should consider. In terms of computational cost, the RSM provides a more efficient alternative to the traditional exhaustive

Table 5. ANOVA for components and their combinations in the CA-Markov model.

Source	Sum of squares	Mean square	F-value	p-value
Model	7.44	0.83	1873.49	< 0.0001
X_1	0.075	0.075	169.83	< 0.0001
X_2	5.25	5.25	11,897.82	< 0.0001
X_3	1.25	1.25	2841.37	< 0.0001
X_1X_2	0.040	0.040	91.79	< 0.0001
X_1X_3	0.021	0.021	48.47	< 0.0001
X_2X_3	0.018	0.018	40.22	< 0.0001
X_1^2	0.12	0.12	275.43	< 0.0001
X_2^2	0.22	0.22	490.77	< 0.0001
$X_1X_2^2$	0.090	0.090	203.16	< 0.0001
R^2	0.9991			

method. For example, using the same spatial scale levels of the three components in the CA-Markov model, the trial number of the RSM is just 26, but there are 50 trials when using the traditional exhaustive method. There is no doubt that the RSM is much more efficient than the traditional exhaustive method, potentially saving considerable time. This is why we used the RSM to explore the spatial scale sensitivity of the CA-Markov model.

5.2. *Impact of spatial scale sensitivity on land use change simulation accuracy*

Because of the unilateral, bilateral, and trilateral effects of cell size and neighborhood size and type on the simulation results as previously discussed, it is critically important to quantitatively understand how much the strength of these component interactions affects the simulation accuracy of the CA-Markov model. According to Equation (4), we developed a third-order polynomial model as follows:

$$\begin{aligned} Y = 1.43 - 0.097x_1 - 0.66x_2 + 0.22x_3 - 0.1x_1^2 + 0.14x_2^2 - 0.14x_1x_2 \\ +0.042x_1x_3 + 0.038x_2x_3 - 0.37x_1x_2^2 \end{aligned} \tag{7}$$

The correlation coefficient (R^2= 0.9991) shown in Table 5 suggests that the equation has a good fit to the individual components and their combinations. The absolute value of a given coefficient in Equation (7) represents the strength at which the individual components or their combinations affect simulation accuracy.

5.2.1. *Individual component impact on land use change simulation accuracy*

As shown in Equation (7), the absolute value of the coefficient of neighborhood size (X_2) is the maximum followed by neighborhood type (X_3), cell number in the neighborhood (X_2^2), cell area (X_1^2), and cell size (X_1). This suggests that changing the scale of the neighborhood size results in the most extreme influence on simulation accuracy. In terms of spatial scale effect, the CA-Markov model is the most sensitive to neighborhood size. Equation (7) shows that cell size, neighborhood size, and cell area are negatively related to simulation accuracy, suggesting that the simulation accuracy increases when the cell size and/or neighborhood size decreases. However, neighborhood type and cell number within the neighborhood are positively related to the simulation accuracy. This suggests that the use of the Von Neumann neighborhood type can achieve better simulation accuracy than that of the use of the Moore neighborhood type. It is particularly interesting that neighborhood size (X_2) and cell number within the neighborhood (X_2^2) have an opposing effect on simulation accuracy. This indicates that it is necessary to maintain a certain cell number within the neighborhood, although a smaller neighborhood size usually results in a better simulation accuracy.

5.2.2. *Component combination interaction impact on land use change simulation accuracy*

The component combination of the CA-Markov model includes bilateral interactions and the trilateral interaction. For the bilateral interactions, Equation (7) shows that $X_2X_3$and$X_1X_3$are positive, but $X_1X_2$is negative. This result suggests that simulation accuracy increases as the cell size and neighborhood size decrease. The absolute value of the coefficients can be sorted in descending order asX_1X_2 (0.14), X_2X_3 (0.042), and X_1X_3 (0.038), whereX_1X_2 is much greater thanX_2X_3 and X_1X_3. This indicates that the bilateral component interaction between the cell and neighborhood size plays a dominant role compared to the other bilateral interactions. This has an important implication, namely that one should pay more attention to the choice of cell and neighborhood size, rather than neighborhood type, during land use change simulation using the CA-Markov model. After all, the bilateral interaction between neighborhood type and cell size or neighborhood size only results in a slight scale effect.

Additionally, we also found another interesting phenomenon as shown in Figure 6(c, d) that no matter whether the cell size is at a fine scale (e.g. 30 m) or a coarse scale (e.g. 150 m), the overall simulation accuracy decreases when the neighborhood size increases. However, the simulation accuracy very slowly decreases at the fine scale, while it rapidly decreases at the coarse scale. This suggests that if the cell size remains constant at a fine scale, the change in the neighborhood size will not lead to an obvious influence on the simulation accuracy. Similarly, if the neighborhood size remains constant at a small scale, the change in the cell size will also not result in a significant effect on the simulation accuracy. However, if the cell size is coarser and the neighborhood size is larger at the same time, the simulation accuracy will worsen. These phenomena are primarily because of the existence of component combination interactions between cell and neighborhood size, which can lessen or enlarge the scale effect from a single component. To achieve a better simulation result of land use change using the CA-Markov model, one must avoid choosing both a coarse scale of cell size and a large scale of neighborhood size.

For trilateral interaction, $X_3$is coded at two levels (−1 and 1) that represent the Moore neighborhood and Von Neumann neighborhood in the central composite design, respectively. BecauseX_3^2equals 1,$X_1X_3^2$and$X_2X_3^2$can be simplified toX_1andX_2, respectively.$X_1X_2^2$ has a negative effect on simulation accuracy. This indicates that simulation accuracy increases as the trilateral interaction decreases. This also requires that the cell and neighborhood size should simultaneously be as small as possible, which is consistent with the single component discussion above. Notably, the absolute value of the coefficient of this trilateral interaction ($X_1X_2^2$) is far greater than that of cell size (X_1). This suggests that their interaction results in a more remarkable scale effect than that of a single cell size. This further indicates that component combination interactions easily result in a more serious influence on land use change simulation than that of an individual component. Therefore, it is necessary to fully understand the component combination interactions to accurately conduct land use change simulation. Our in-depth exploration of the spatial scale sensitivity of the CA-Markov model sheds some light on this issue.

6. Conclusions

The spatial scale sensitivity of the CA-Markov model for land use change simulation, which mainly originates from cell size, neighborhood size, and neighborhood type, is very complex. It leads to obvious impacts on the accuracy of land use change simulation.

This study has made use of the RSM to comprehensively explore the scale sensitivity of the CA-Markov model via individual components and their combinations. The main conclusions can be summarized as follows:

(1) The CA-Markov model is significantly sensitive to spatial scale change via individual components as well as their combinations. Furthermore, the presence of component combination interactions easily leads to uncertainty in land use change simulation, similar to individual components.
(2) The utility of our proposed hybrid evaluation model and the RSM to explore the spatial scale sensitivity of the CA-Markov model has proven to be more accurate than that of the single Kappa coefficient evaluation index and more efficient than that of the traditional methods (e.g. the traditional exhaustive and orthogonal test methods). A thorough analysis has demonstrated the superiority of the hybrid evaluation model in terms of accuracy and the RSM in term of efficiency.
(3) Considering individual component effects, the CA-Markov model is more sensitive to neighborhood size than cell size or neighborhood type. Undeniably, the bilateral and trilateral interaction between neighborhood size and cell size results in a more marked scale effect than cell size alone. When conducting a land use change simulation using the CA-Markov model, one should maintain a certain cell number within the neighborhood and avoid choosing both a coarse scale of cell size and a large scale of neighborhood size.

Despite the achievements in this study, there are several aspects that warrant further investigation, particularly when various transition rules (e.g. neural network, genetic algorithm, and ant colony optimization) are available. Given the difference in these transition rules, it is also essential to seek an appropriate method with which to examine their spatial scale sensitivities as soon as possible. However, one should pay more attention to spatial pattern differences from various study areas in future studies, although distinctive land use patterns from a certain study area do not have the universal feature of spatial scale sensitivity, thus that we cannot attribute it to an internal factor of the CA-Markov model.

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