

Neural Cellular Automata-based Land Use Changes Simulation

Jinian Zhang^{1,2}, Lanfa Liu^{1,2}

¹ College of Urban and Environmental Sciences, Central China Normal University,
Wuhan, China-ccnuzjn2023@mails.ccnu.edu.cn, lanfa@ccnu.edu.cn

² Hubei Provincial Key Laboratory for Geographical Process Analysis and Simulation,
Central China Normal University, Wuhan, China

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Abstract

Simulating land use and land cover changes (LUCC) is important for urban planning and environmental studies. In this study, we introduce a neural cellular automata (NCA) model that integrates biological principles and convolutional neural networks (CNNs) for land use simulation. We conduct experiments in the city of Wuhan, China. The NCA model achieved the highest performance with an OA of 0.858, F1 score of 0.753, Kappa coefficient of 0.799, and FOM of 0.427. Comparisons of land use data of Wuhan city from 2000 and 2010 with the simulated optimal results indicate that forest areas closer to urban centers are more susceptible to modernization processes, showing the advantage of NCA in accurately simulating land use changes in the central urban area.

1. Introduction

Land use and land cover changes (LUCC) is an important component of Earth system dynamics that not only alters biophysical surface characteristics (Homer et al., 2020) but also has significant impacts on the environment in terms of climate, hydrological systems, biodiversity, ecosystem services, etc (Chai and Li, 2023). The mechanism of LUCC is extremely complex, and it is useful to take advantage of simulation models to understand the driving factors and to project future land use changes (Xu et al., 2021).

Land use simulation models are developed to project future land use consumption under different scenarios. Conversion of Land Use and its Effects Model (CLUE) is a model used to simulate and analyze land use changes and their environmental impacts, focusing on how to integrate the effects of multiple drivers. As a spatial version of CLUE, CLUE-S achieved good results in applications in Europe (Wu et al., 2022a). However, there are still some shortcomings in the measurement of process effects and the balance of land supply and demand. Agent-Based Model (ABM) provides a way to simulate the behavior and interaction of individuals or agents from a microscopic perspective. This model is particularly useful for studying the complex interactions between human activities and the natural environment, and how these interactions influence changes in land use patterns. The model takes into account interactions between macro (environmental) and micro (human) factors, without interactions between human agents (Xu et al., 2020).

Cellular Automata (CA) is one of the most popular models adopted for LUCC simulation (Zhai et al., 2020). CA is a discrete dynamic system, which consists of a rule, grid, cells, and states. Each cell is in a finite set of states. This state changes over time, and the change is controlled by the state of the cell itself and the states of its surrounding neighbor cells. The essence of the CA simulation model is that it uses simple transform rules to change the local state, thereby changing the global state (Liu et al., 2023). CA applies simple interaction rules at a local level and can simulate very complex and unpredictable system behavior (Jumba and Dragičević, 2016). Therefore, CA has become

a powerful tool for modeling and understanding the dynamic behavior of natural and artificial systems (Siddiqui et al., 2018).

Previous research has explored various methods to enhance the performance of CA models. Improvements have been made at the cell and grid levels, developing CA based on land natural evolution unit (Xu et al., 2023) and urban Vector-based CA (Li et al., 2017). The transition rule is at the core of the CA model, which determines how a cell updates its state based on the current states of itself and its neighbors. The logistic regression method (Wang et al., 2021) leverages statistical techniques to model the relationship between input variables and land use changes, providing valuable insights into the driving factors of LUCC. Markov model (Subedi et al., 2013) utilizes transition probabilities to predict future land use based on historical data, making them particularly useful for long-term forecasting. Heuristic algorithm (Feng et al., 2011) and random forest algorithm (Kamusoko and Gamba, 2015) excel at handling complex datasets and nonlinear relationships, enhancing the predictive power of CA models in dynamic environments. Artificial neural networks (ANNs) (Fei He and Xia, 2022) offer the ability to capture intricate patterns and dependencies within data, allowing for more nuanced predictions. Patch-generating land use simulation (PLUS) model (Liang et al., 2021) integrates a land expansion analysis strategy and multi-type random patch seeds to understand the drivers of land expansion. Integrating these methods with CA further enhances model performance by leveraging the strengths of each approach while mitigating their limitations.

LUCC is a nonlinear process involving complex connections and feedback between land use and driving factors with spatial correlation effects (Geng et al., 2022). It is difficult to comprehensively analyze the driving mechanism of LUCC using the traditional CA model. In the past few years, researchers have gradually begun to shift their attention to deep learning due to the great development of large datasets and computer technology. The deep learning framework excels in exploring deep relationships between underlying factors (LeCun et al., 2015). Convolutional neural networks (CNNs) as a typical deep learning method is suitable for processing high-dimensional data by

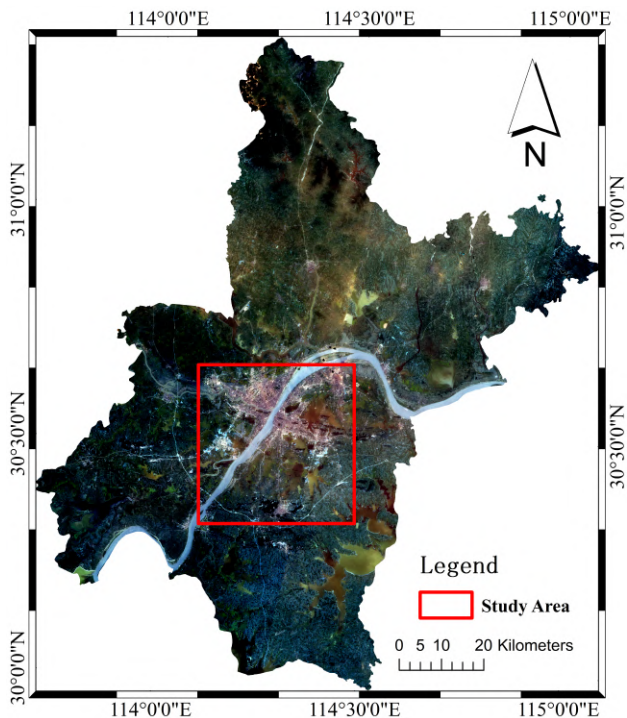


Figure 1. Location of study area in the city of Wuhan, China

adopting convolutional operations to extract features from input data. The structure is flexible to different tasks and data to achieve better performance. When processing data with spatial characteristics or involving image information processing, CNN can capture the spatial dependence within the data by taking advantage of its hierarchical structure of convolutional layers (Wu et al., 2022b). Neural Cellular Automata (NCA) (Mordvintsev et al., 2020) is proposed to create a self-repairing system that emulates biological properties. NCA is based on biological principle that cells often rely only on chemical gradients to guide the organism's development and the principle that they renew themselves at regular intervals, using CNN to extract transform rules.

The aim of the present paper is to explore the potential of NCA for land use changes simulation. In NCA, the Sobel filter is adopted to calculate the perception of the central cell from land-use data and driving factors, and convolutional layers with different sizes of kernels are considered to extract the transform rules for the simulation. We perform experiments in urban area of Wuhan city in China with relevant factor data. The model takes advantage of biology knowledge and shows strong advantages in digging deep information and self-learning.

2. Materials

2.1 Study Area

Wuhan City is located at longitudes 113°41' to 115°05' East and latitudes 29°58' to 31°22' North, in the eastern part of Hubei Province, China. It is situated at the confluence of the Yangtze River and Han River, making it a vital transportation hub in the central region of China, serving as a crucial link connecting the eastern coastal region and the western inland provinces. Wuhan City is not only the political, economic, and cultural center of Hubei Province but also one of the core cities of the Yangtze River Economic Belt. In recent years, it has

Factors name	Source
DEM	ASTER Global Digital Elevation Map (https://asterweb.jpl.nasa.gov/gdem.asp)
Slope	Derived from DEM
Distance to water	Derived from land-use data
Population	WorldPop(https://www.worldpop.org/)
Distance to railway	OpenStreetMap (https://www.openstreetmap.org/)
Distance to expressway	OpenStreetMap (https://www.openstreetmap.org/)
Distance to national highway	OpenStreetMap (https://www.openstreetmap.org/)

Table 1. Impact Factors and Their Source

developed rapidly and become an important driving force for regional economic development. The urban building complex in the center of Wuhan and its surroundings are selected as the research area (Figure 1).

2.2 Data Source

In this study, land-use data from GlobalLand30 is considered for the period of 2000 to 2010. The Globalland30 dataset is a high-resolution global land cover dataset developed by the State Key Laboratory of Resources and Environmental Information System at the Chinese Academy of Sciences. It utilizes time-series Landsat data and other ancillary data to generate land cover classifications using a 10-category classification system, providing 30-meter resolution land cover information across the entire globe. The Globalland30 dataset has been widely applied in various fields, including land use and land cover change research, climate change studies, and natural resource management. GlobalLand30 data is obtained from PIE-Engine (<https://engine.piesat.cn/>).

A range of natural and socioeconomic factors listed in Table 1 are chosen including DEM, slope, distance to water, population, distance to railway, distance to expressway, and distance to national highway. DEM and slope factors reflect the topographic characteristics of the study area, which influence the spatial distribution patterns of human activities and consequently the spatial patterns of land cover change. The distance to water bodies is a crucial determinant of the distribution and change of the agricultural land. Population density is a key socioeconomic factor that reflects the intensity of human activities within a given area. Proximity to transportation infrastructure greatly influences accessibility and connectivity, facilitating the movement of people, goods, and resources. These factors are resampled to a uniform spatial resolution of 30 meters and normalized as shown in Figure 2.

3. Methodology

3.1 Structure of NCA

The structure of NCA is shown in Figure 3. It can be divided into two parts: the perception part and the rule-learning part. The perception part describes each cell's perception of the surrounding area. We use the Sobel filters to calculate the perception matrix. The Sobel filter, also known as the Sobel operator, is a discrete differentiation operator with the advantage

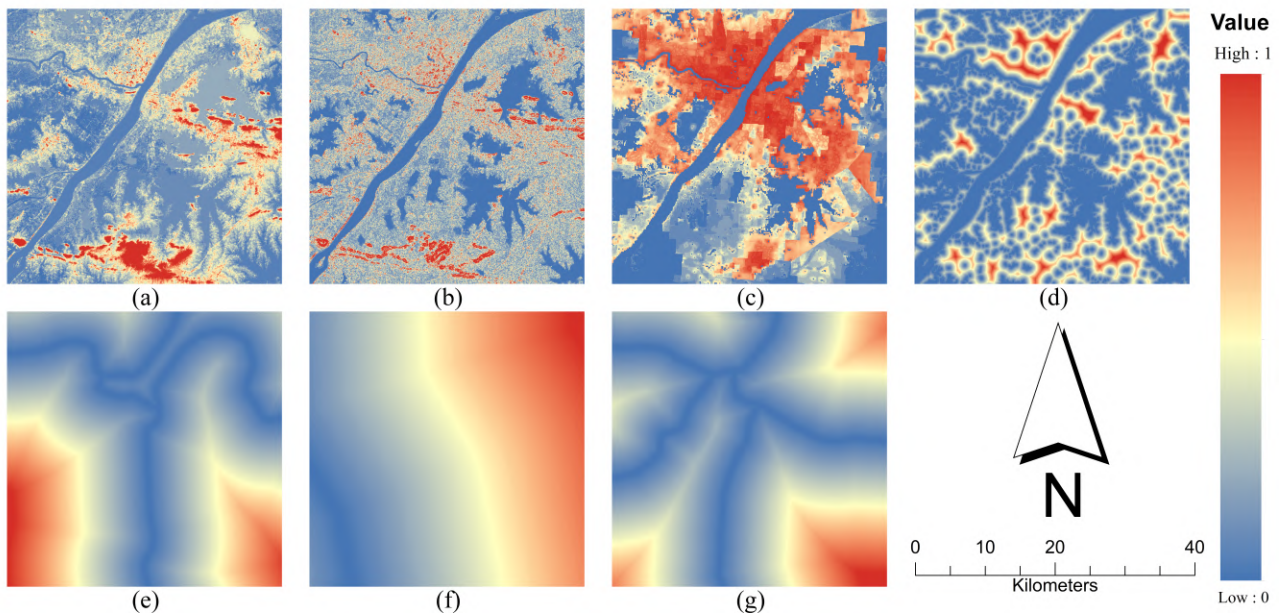


Figure 2. Collected factors of Wuhan city in this study. (a) DEM. (b) Slope. (c) Population. (d) Distance to water. (e) Distance to railway. (f) Distance to expressway. (g) Distance to national highway.

that it combines Gaussian smoothing and differential derivation, which can reduce the impact of noise. In this part, it is used to smooth errors in input data and calculate the perception value of the central cell in horizontal and vertical orientations. Then, we concatenate the perception matrix with the input data and feed it into the next section.

The second part is to obtain the transform rules. Six combinations of convolution layers with ReLU activation are employed. The combination is often used to capture local information from the input data. Specifically, the first four convolutional layers have a kernel size of 3, aiming to extract information from around the central pixel. The subsequent two convolutional layers have a kernel size of 1, achieving the effect of a fully connected layer.

By leveraging the strengths of convolutional neural networks and incorporating spatial context through the perception matrix, NCA can effectively capture the complex interactions and dependencies within the land use data.

3.2 NCA for Land Use Simulation

As depicted in Figure 4, the training of land use change using NCA involves three steps: data preparation, model training and evaluation using validation samples. Firstly, land-use data and seven factors obtained from different sources are stacked to obtain the 8-band input data. Then, data augment is performed through random angle rotation and random mirror flip to improve the generalization ability of the model, reduce overfitting and enhance the robustness. After that, the input data is split into training and validation samples at a ratio of 8:2. For the training step, data is ingested into the model to obtain the output, and then determine whether the simulation is complete based on the number of iterations. The model is trained using the backpropagation method. The final step involves evaluating performance using validation samples using several metrics.

It is necessary to set the number of simulation iterate times before training the model, which is related to the simulation

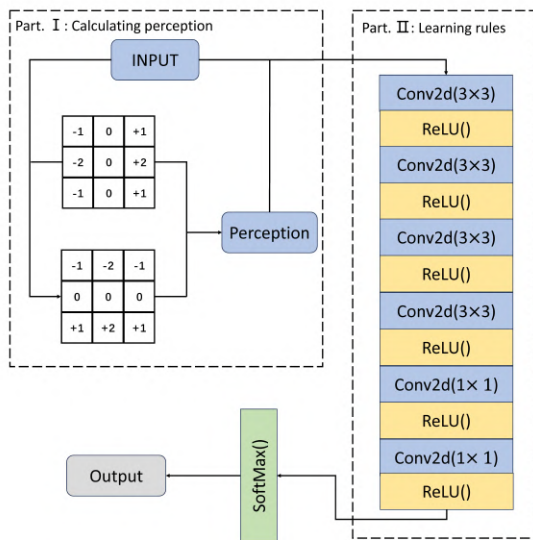


Figure 3. Structure of NCA. In the first part, the perceptual matrix is calculated using the Sobel filter and fed into the next part along with the input data. The second part uses multi-layer convolution and activation to extract transformation rules.

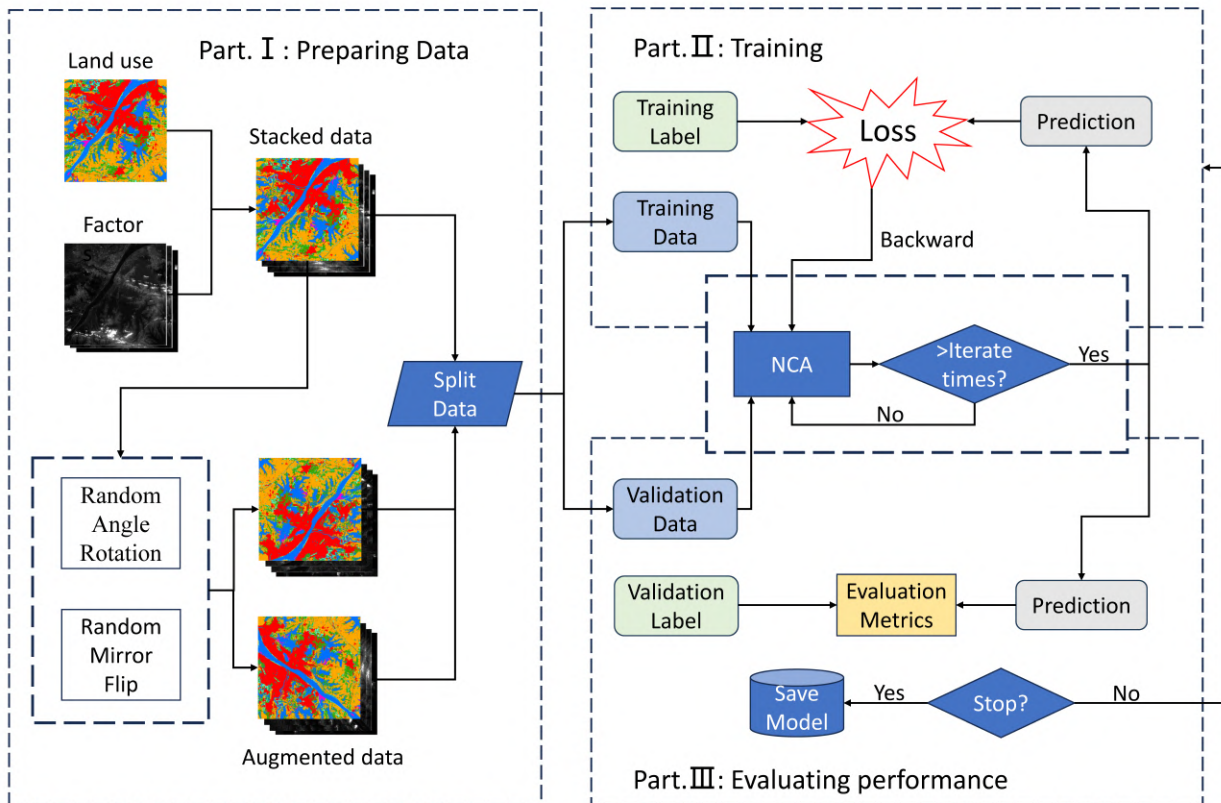


Figure 4. Workflow using NCA for land use change simulation.

interval. For example, the present study investigates land use changes in Wuhan city from 2000 to 2010 with a period of ten years. The period is divided into different intervals, such as 1 year, 2 years, 5 years, or 10 years, with each interval considered as a cycle. A cycle of 1 year means that 10 iterate times need to be performed.

The experimental environments are NVIDIA GeForce GTX 1660Ti, Python3.9, and PyTorch 1.12.0. During the training process, we set hyperparameters as follows: the optimizer in all the experiments is Adam, the batch size is 4, the epoch is 300, and the learning rate is initially set to 0.0001 and adjusted in different experiments.

3.3 Model Evaluation

The overall accuracy (OA), F1 score, Kappa coefficient, and Figure of Merit (FOM) are used to evaluate the NCA model. OA is the most common metric used to evaluate land use change models. It calculates the proportion of all correctly predicted samples to the total number of all predicted samples, ranging from 0 to 1. F1 score considers both precision and recall of the model. The F1 score was originally designed for binary classification problems but can be extended to multi-class classification problems. F1 score can be calculated on each class and then take the average as the overall performance metric. This approach is known as the macro-average F1 score, which is the case in our study. It also ranges from 0 to 1, where a value closer

to 1 indicates better performance of the model. The formula for OA and F1 score are:

$$OA = \frac{TP + TN}{TP + TN + FP + FN} \quad (1)$$

$$F1 = \frac{2 \times TP}{2 \times TP + FP + FN} \quad (2)$$

where TP (True Positives) represents that the model correctly predicts the positive class; TN (True Negatives) represents the model correctly predicts the negative class; FP (False Positives) represents the model incorrectly predicts the positive class when it's actually negative; FN (False Negatives) represents the model incorrectly predicts the negative class when it's actually positive.

The Kappa coefficient is a metric that shows the relationship between the simulation results and the ground truth. The calculation of the kappa coefficient is based on the confusion matrix and the value ranges from -1 to 1. Typically it is greater than 0. The closer the value to 1 means the better the simulation performance (Monserud and Leemans, 1992). The formula for Kappa is:

$$Kappa = \frac{P_o - P_e}{1 - P_e} \quad (3)$$

$$P_e = \sum_{i=1}^n \frac{(\sum_{j=1}^n x_{ij})(\sum_{j=1}^n x_{ji})}{(\sum_{i=1}^n \sum_{j=1}^n x_{ij})^2} \quad (4)$$

$$P_o = \frac{\sum_{i=1}^n x_{ii}}{\sum_{i=1}^n \sum_{j=1}^n x_{ij}} \quad (5)$$

where P_o represents observed agreement probability, reflecting the frequency of correct predictions; P_e represents the expected consistency probability, which reflects the probability that the prediction result is consistent with the true label under random prediction; i and j respectively represent the rows and columns of the confusion matrix; x_{ij} represents the element in the i -th row and j -th column of the confusion matrix.

FOM measures the consistency between simulated changes and actual changes, ranging from 0 to 1. A value closer to 1 indicates better simulation performance (Pontius et al., 2008). The formula for FOM is:

$$FOM = \frac{B}{(A + B + C + D)} \quad (6)$$

where A represents the number of pixels where there is a change in ground truth but the simulation remains unchanged; B denotes the number of pixels where both ground truth and simulation changed and the change is correct; C signifies the number of pixels where both ground truth and simulation changed, but the change is incorrect; D stands for the number of pixels where there is a change in simulation but the ground truth remains unchanged.

4. Results

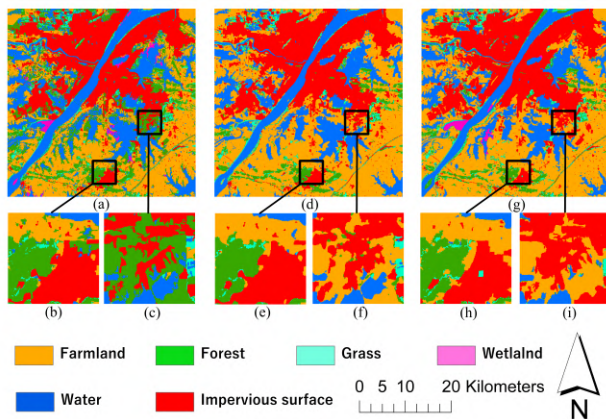


Figure 5. Comparison of land use in 2000, simulation in 2010, and reference in 2010. (a), (d), and (g) are land-use in 2000, the simulation result, and land-use in 2010, respectively. (b), (e), (h), and (c), (f), (i) are the magnified details of the areas far and near from the central urban building complex, respectively.

Figure 5 illustrates land use in 2000, 2010, and simulated 2010 data in Wuhan City under the setting of iterate times as 1. Generally, forested areas closer to urban centers appear to be more susceptible to modernization processes. The simulation correctly reflects forest degradation in proximity to cities. More specifically, (c), (f), and (i) depict the perimeters of the central urban building complex in Wuhan city. It is evident that the majority of forests have undergone degradation. In contrast, forests in (b), (e), and (h) situated away from the central city buildings show minimal change or remain relatively unchanged.

In this study, the effect of iterate time is explored by setting to 1, 2, 5, and 10 times, corresponding to simulations conducted over periods of 10, 5, 2, and 1 year respectively. The quantitative evaluation results for the four settings are presented in Table 2. As the number of iterate time increases, OA, F1 score, Kappa, and FOM show a downward trend, indicating a decline in the performance of NCA. Specifically, when the number of iterate time is 1, OA reaches 0.858, F1 reaches 0.753, Kappa reaches 0.799, and FOM reaches 0.427, making it the best-simulated performance of NCA among the four settings.

Iterate time	OA	F1 score	Kappa	FOM
1	0.858	0.753	0.799	0.427
2	0.834	0.635	0.765	0.388
5	0.672	0.459	0.521	0.239
10	0.653	0.430	0.496	0.239

Table 2. Evaluation Metrics for NCA Simulation Results

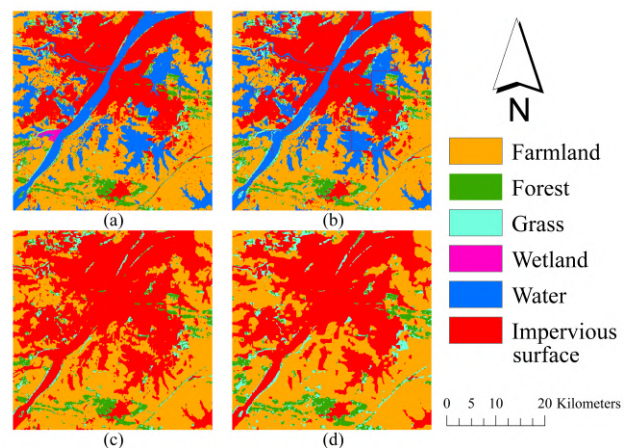


Figure 6. Comparison of results of different iterate times. (a), (b), (c), and (d) respectively represent the results for iterate times set to 1, 2, 5, and 10.

Figure 6 shows the results under four settings. Consistent with the performance metrics, when the number of iterate time is set to 1, the simulation results are most reasonable. However, with iterate time setting as 2, some errors exist but the overall simulation result is acceptable. In contrast, with iterate time setting as 5 or 10, the performance of NCA is poor and fails to accurately simulate the changes of water and impermeable surfaces. In summary, when the value of iterate time is set as 1, the NCA model achieved the best land use changes simulation result.

5. Conclusion

In this study, we present the NCA model for land use changes simulation using GlobalLand30 dataset and factor data from different sources. Based on the biological principle that cells alter their states according to the surrounding environment and regularly self-update, NCA calculates and incorporates the perception vector as part of the network's input, which allows the CNNs to extract the transform rules for cellular automata, enabling the simulation of land use change in the study area. This method combines the characterization of local interactions by cellular automata and the powerful feature extraction capability

of convolutional neural networks, providing a novel and effective approach for land use change simulation. The results show that NCA performs well in simulating land use changes in different regions under the background of urbanization.

Acknowledgments

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