Simulating mixed land-use change under multi-label concept by integrating a convolutional neural network and cellular automata: a case study of Huizhou, China

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ABSTRACT

Cellular automata (CA) model is a useful tool for simulating spatiotemporal changes of land-use evolution. However, previous CA models have usually ignored the inhomogeneous and mixed land-use situations and simplified the land grid cell as one single land-use type. This study developed a multi-label (ML) convolutional neural network CA (ML-CNN-CA) model to simulate the complex evolution of mixed land uses. The multi-label learning strategy in the proposed model can formulate mixed land uses by labeling multiple land-use types to each grid cell. The transition rules of CA were modified to accommodate the multi-label learning strategy and mined by coupling a CNN network and three interactive mechanisms, including the neighborhood effect, adaptive inertia coefficient, and random factor. The proposed ML-CNN-CA model was applied and examined in a fast-developing city (Huizhou) in the China's Pearl River Delta region for the mixed land-use simulation during 2009–2013 and 2013–2020. The ML-CNN-CA model with different CNN architectures and a previous artificial neural network (ANN)-based multi-label CA model were also implemented for comparisons. Results show the capability of the ML-CNN-CA model to simulate fine-scale mixed land-use changes with satisfactory performances. Specifically, the simulated mixed land-use patterns agree well with the actual land uses from the morphological perspective. Furthermore, the quantitative assessments demonstrate the performance of the proposed model, showing an accuracy value of 0.912 for 2009–2013 and 0.896 for 2013–2020, and a hammering loss value of 0.048 for 2009–2013 and 0.055 for 2013–2020. The comparisons also show the best performance of the ML-CNN-CA model with the VGG-based architecture and significant outperformance of the proposed model against the previous ANN-based CA model. Multiple sensitivity analyses were also conducted to investigate the uncertainty of the proposed model. The ML-CNN-CA model proposed in this study can provide a new tool for better simulation of fine-scale mixed land-use changes and is expected to help formulate urban planning guidelines and achieve sustainable urban development.

1. Introduction

Land-use change modeling is crucial for investigating the profound impacts of land-use dynamics on various aspects of the natural and social environment, including climate change, biological diversity, energy consumption, and human activities (Chen et al. 2020; Güneralp et al. 2017; Faisal et al. 2021; Kafy et al. 2021; Li et al. 2017; Mantyka-Pringle et al. 2015; Pielke 2005). With unprecedented global urbanization to date, land-use change models can provide valuable guidance for understanding the complex urban land-use system and its dynamics, thus supporting land-use management and sustainable urban development (Li et al. 2017; Paulit, Ennos, and Golding 2005; Verburg et al. 2004). As one of the most popular land-use change simulation models, cellular automata (CA) has been widely used to capture and simulate the spatiotemporal land-use dynamics for diverse regions or scales (Clarke and Gaydos 1998; Li and Yeh 2002; Liu et al. 2017; Van Vliet et al. 2012; White and Engelen 1993; Wu and Martin 2002). By considering various driving factors related to urban development, land-use initial state, neighborhood cellular effects, and different transition rules as integrations, CA models can capture the spatial details and characterize the stochastic land-use change process (Santé et al. 2010). Although simple in principle, CA has demonstrated a strong capability for understanding urban dynamics. Thus, CA models have been widely used in land-use change modeling and further applied in various urban studies (Chen et al. 2016; Kafy et al. 2021; Liang et al. 2018; Liang et al. 2018; Zhang et al. 2020).
As the basic units in the CA model, the land-use cells are usually assumed and allocated within a single or discrete land-use type or state for the simulation (Liu et al. 2010; Qian et al. 2020; Yeh and Li 2006). However, land-use units could generally involve multiple land-use types (e.g. an urban cell may contain residences and industrial sites) or inhomogeneous land structures (Liu et al. 2018; White, Ulijee, and Engelen 2012). The accelerated urbanization and continuous land development in the past decades have led to increased intensity and complexity of land-use structures, especially in dense urban areas (Tayyebi and Pijanowski 2014; Verburg et al. 2009). For example, the land space is increasingly planned or used as multiple parts to serve the diverse land functions for cities. Although the inner change in land-use mix improves land-use efficiency and thus promotes compact city development, it has a significant impact on a wide range of urban environmental and social issues, such as on energy consumption (Woo and Cho 2018) and human mobility (Yue et al. 2017), thereby profoundly affecting urban sustainability. Hence, modeling the dynamics of mixed land-use evolution can provide more realistic guidance for planners and be further applied to various urban studies and land management under the complex land system (Song and Knaap 2004; Stevenson et al. 2016; Yue et al. 2017). However, the traditional CA models assume that one single land-use type in each grid cell can be insufficient to model the complex land system under the growing mixed land-use scenario in reality.

Capturing the mixed land-use dynamics is more complex than modeling the traditional pure-cell-based land-use change. Specifically, for mixed land-use change modeling, the land-use units have multiple-land components with highly nonlinear and spatially stochastic interactions that may be related to various social, environmental, and planning factors (Abdullahi et al. 2015). Only a few studies have attempted to analyze or model complex mixed land-use changes in recent years. Specifically, they can be mainly summarized into two categories, including models based on the proportions of land-use components and models based on the multilabel concept. Liang et al. (2021) developed a mixed-cell CA model to simulate mixed land-use change by modeling the basic land-use cell with the proportions of multiple land-use components. The transition rules for the mixed-cell CA model were intelligently mined and constructed based on the cell, neighborhood, and sub-cell scales to formulate dynamic interactions of mixed land uses. According to the re-defined evaluation methods, the mixed-cell CA model has achieved satisfactory simulation accuracies and demonstrated the practicability of future mixed land-use change projections in a metropolitan area. However, because of the precise proportions modeling for each mixed land-use cell defined in the model, the mixed-cell CA simulation can lead to a substantial computational cost, especially for large-scale applications. In addition, with the development of machine learning, multilabel (ML) learning, as an emerging paradigm, provides simple, flexible, and efficient representations to achieve mixed land-use modeling by assigning multiple states to each instance in CA (Grigoris and Ioannis 2007; Zhang and Zhou 2014). In contrast to traditional classification tasks where labels are mutually exclusive, multi-label paradigms support the modeling of nonexclusive labels (Zhang and Zhang 2010). Thus, based on the concept of multi-label learning, multiple land-use types in CA can be formulated as a set of labels for each cell and subsequently accommodated to different land-use modeling methodologies. Existing studies have verified that integrating the multi-label concept in land-use change modeling can effectively model and simulate mixed land-use evolution (Omrani et al. 2015). By accommodating the multi-label concept, relevant ML-CA models were developed by mining the transition rules with the advanced machine learning approach (e.g. the Rank-Support vector machine (SVM) and artificial neural networks (ANNs)) (Charif et al. 2017; Omrani, Tayyebi, and Pijanowski 2017), which further demonstrated the outperformance of mixed land-use change simulation of the multi-label model compared to mono-labeling modeling (Omrani, Tayyebi, and Pijanowski 2017).

Although multi-label learning provides a more flexible and appropriate paradigm for CA modeling, further improvements and applications are needed to achieve accurate mixed land-use change simulations. For example, the nonlinear relationship between mixed land-use change and various spatial driving factors is more complex than the traditional pure-CA model (e.g. mapping the relationship between various driving factors to multiple land-use types within a cell) due to the high-dimensional
output label space. In addition, the transition rules of CA modeling under the multi-label concept have not been sufficiently mined in previous studies, which can be limited to representing the complex inner competitions and interactions of mixed land-use dynamics.

In this study, we developed a CA model (ML-CNN-CA) under the multi-label concept to simulate the mixed land-use evolution. The model’s main assumption is to assign multiple land-use types to each land-use cell, thus allowing mixed land-use conversion within a cell. To capture the complex mixed land-use dynamics, we adopted a deep-mining strategy and an interactive mechanism by integrating specific CNN networks and intelligent CA modules as the CA transition rules for the simulation. In particular, Convolutional neural networks (CNNs) in particular have been shown to perform well in automatically extracting discriminative features from multiple spatial driving factors, demonstrating their functionality in CA simulation (He et al. 2018; Zhai et al. 2020). Hence, we used a specific CNN network (VGG-Net) to excavate the multidimensional relationship between various spatial driving factors and derive land-use suitability for mixed land uses. Furthermore, we integrated three interactive modules, including neighborhood effects, adaptive inertia coefficients, and random factor, along with the land-use suitability to determine the transition rules of CA model, where all these modules were re-designed based on multi-label learning. To verify the effectiveness of our model, we applied the proposed CA model with rich spatial data in Huizhou, a fast-developing city in the Guangdong-Hong Kong-Macao Greater Bay Area, China, for simulating the mixed land-use change of 2009–2013 and 2013–2020. We further evaluated the model performance based on accuracy assessment, spatial pattern inspection, and model comparison. Moreover, to understand the different influences of configurations on the simulation results, we investigated the model sensitivity on varying parameter settings and the importance of the selected driving factors. Our specific research objectives of this study were to: (1) propose a modified CA model to model the complex dynamics of mixed land use; (2) apply the proposed model with rich city data to simulate the mixed land-use change of a fast-developing city and verify its effectiveness; (3) investigate the uncertainty of the proposed model for urban mixed land-use change simulations.

2. Methodology

Here, we developed a CNN-based CA model (ML-CNN-CA) to simulate mixed land-use changes under the multilabel concept. Figure 1 illustrates the overall framework of the ML-CNN-CA model. Similar to the framework of the traditional CA model, the ML-CNN-CA model mainly contains two components: (1) mining the non-linear interactions between spatial driving factors and the change of mixed land-use label within a basic unit; and (2) defining appropriate CA transition rules under a multilabel paradigm for mixed land-use change simulation. In particular, we used a compact visual geometry group (VGG)-based CNN network to deal with the complex relationships between driving factors and mixed land-use labels, resulting in multi-label land-use development suitability. Specifically, land-use development suitability is an approximate proxy that reflects the probability of land-use occurrence within a cell, which is generally derived based on various spatial driving factors. By integrating the development suitability, neighborhood effects, adaptive inertia coefficients, and random factor as the transition rules, the overall transition probability is obtained to determine the internal mixed land-use conversion. In our model, all modules were redesigned using multi-label learning to allow land-use conversion for multiple land-use types within a basic unit. As the final step, an adaptive threshold was adopted to control the overall conversion and a constraint matrix was built based on historical mixed land-use change trends for achieving more realistic simulation. In the following sections, we introduce the principle of the ML-CNN-CA model and the corresponding evaluation indicators for the model performance.

2.2. Specific CNN framework

The process of land-use evolution is highly relevant to a series of driving factors of urban development, such as urban planning, traffic, and environmental aspects (Santé et al. 2010). Previous studies have adopted different intelligence algorithms to determine land-use suitability in CA models, such as the Artificial Neural Network, Radom Forests (Gounardis et al. 2019; Shafizadeh-Moghadam et al. 2021), Support Vector Machine (Yang, Li, and Shi 2008), etc. In our modeling framework, the spatial drivers are employed
to mine and further derive mixed land-use suitability for independent labels within each land-use cell. To this end, mining the relationship between spatial drivers and mixed land-use change could be more challenging under the multi-label concept due to many factors such as high dimensionality, unbalanced data, and the huge number of labels combinations (Alazaidah and Kabir 2016). Existing studies have demonstrated that the convolutional neural networks (CNNs) have achieved state-of-the-art performance in addressing the challenges of multi-label tasks (Wei et al. 2014, 2016; Zeggada, Melgani, and Bazi 2017). Thus, we adopted a compact VGG network (Figure 2) modified from VGG-16 (Simonyan and Zisserman 2014), one of the most commonly used CNN architecture for its effectiveness, to extract significant features and obtain mixed land-use development suitability for further modeling.

Figure 2 illustrates the architecture of the VGG-based network used in this study. In particular, the structure of the VGG-based network contained five one-dimensional convolutional layers, three max-
pooling layers, and two fully connected layers. We set the repeated convolutional layers to size three in the network to enhance the ability to learn the spatial features after a series of non-linear transformations. Additionally, the max-pooling layers of size 2 are applied to reduce the model parameters, while the probabilities of dropping neurons are set as 25% and 50% to avoid overfitting problems. At the end of the network, we adopted two fully connected layers to flatten the extracted features and then took the output of the previous layers corresponding to the multiple land-use labels. The advantage of the VGG-based network is that it can take full advantage of the convolution and pooling layers of the network to generate high-level class-specific features without increasing the complexity of the network architecture (He et al. 2021; Lydia and Francis 2020). Meanwhile, VGG-based networks with similar compact architectures as this study have been applied to different scenes and validated their effectiveness in multi-label classifications (Hua, Mou, and Zhu 2019; Li et al. 2020).

2.3. A modified multi-label cellular automata model

To simulate land-use evolution, CA models commonly assume and estimate the state of the cell according to its initial conditions, the surrounding neighborhood effects, and a series of transition rules, which are aggregated as the overall transition probability (Santé et al. 2010). Based on the principle of traditional CA models, we further integrated the development suitability (PG), neighborhood effect (Ω), self-adaptive inertia coefficient (I) and the random factor (R) as the overall transition rules of our modified CA model for mixed land-use simulation. As one of the critical components of land-use dynamics, proximity reflects the impact of the surrounding land resource configuration on land-use evolution within a unit, which is generally modeled as the neighborhood effect in CA (Dahal and Chow 2015). This study used the most typical neighborhood, the Moore neighborhood (i.e. \( n \times n \) grid window), to derive the neighborhood effect in our CA model. However, in contrast to the traditional neighborhood effect modeling that shares equal surrounding impacts, mixed land use have led to inhomogeneous neighborhood influence during its evolution. For example, a mixed land-use cell with labels of “urban” and “industry” has different neighborhood effects compared to a pure cell with an urban label. Therefore, to accurately evaluate the impact of surrounding mixed land-use types on the central cell, we modified the calculation of the neighborhood effect. We assumed \( N \) is the number of land-use cells of a city, and \( x_i (i = 1, 2, \ldots, N) \) refers to each land-use unit. \( M \) represents the total categories of land uses, and each \( x_i \) is allocated to the land-use labels with one-hot encoding as \( y_i = [y_{i1}, y_{i2}, \ldots, y_{iM}] \).

Thus, \( S_{j_i} = \sum_{j=1}^{M} y_{ij} \) represents the number of land-use labels in a cell. The Moore neighborhood of \( x_i \) is defined as \( C_{x_i} \), which is \( n \times n \) windows, and \( W_{j_i} = \frac{y_{ij}}{S_{j_i}} \) is used to estimate the influence of \( y_i \) with its corresponding labels at the interaction time \( t \). For example, the labels \( y_i \) of the grid cell \( x_i \) at time \( t \) are \([1,0,0,1]\) and, thus, the \( S_{y_i} = 2 \). In this case, the \( W_{y_i} = [\frac{1}{2},0,0, \frac{1}{2}] \) according to the formula defined previously. Thus, the modified neighborhood effects can be estimated using the following equation:

\[
\Omega_{x_i}^{t} = \frac{\sum_{x_k \in C_{x_i}} W_{j_k}}{n \times n - 1}
\]

Here, \( \sum_{x_k \in C_{x_i}} W_{j_k} \) represents the total effects of the surrounding pixels on the central grid cells \( x_i \) on each land-use label in Moore neighborhood \( C_{x_i} \) at time \( t \). Thus, the inhomogeneous neighborhood effect is determined by considering the number of labels as the degree of the mixture within a land-use cell.

In addition, as an auto-adjustment mechanism, the self-adaptive inertia coefficient is defined and adopted in CA models to adjust the land-use change rates and facilitate convergence to the expected quantity (Li et al. 2017; Liu et al. 2017). We further integrated this coefficient into the transition rules to help model the complex competitions and interactions among mixed land-use changes. In this mechanism, a self-adaptive inertia coefficient for each land-use label is defined to automatically adjust the conversion probability of current land uses on each cell according to the differences between the macro label and the allocated label demand at time
t. For example, suppose the developing trend of a specific land-use type contradicts the macro demand. In that case, the inertia coefficient dynamically increases the inheritance of this land-use type and rectifies the development trend of land-use change in the next iteration. Based on the preceding definitions, \( Y = \sum_{i=1}^{N} y_i \) is introduced as the amount of each allocated label for all land-use cells at iteration time \( t \), such as the count of the label “urban.” Therefore, the inertia coefficient is defined as:

\[
\begin{align*}
I_y^t &= \begin{cases} 
I_y^{t-1} & \text{if } |D_y^{t-1}| \leq |D_y^{t-2}| \\
I_y^{t-1} \times \frac{D_y^{t-2}}{D_y^{t-2}} & \text{if } D_y^{t-1} < D_y^{t-2} < 0 \\
I_y^{t-1} \times \frac{D_y^{t-2}}{D_y^{t-1}} & \text{if } 0 < D_y^{t-2} < D_y^{t-1}
\end{cases}
\] (2)

where \( I_y^t \) represents the inertia coefficient of the allocated land-use labels at iteration time \( t \), \( D_y^{t-1} \) represents the difference between the current and target land-use labels at iteration time \( t - 1 \), and the coefficient is initially one. Moreover, given that land-use evolution is a complex process and is usually influenced by stochastic factors (Wu and Martin 2002), we coupled the random factor to control the effect of the stochastic perturbation on our model. Here, the random factor can be expressed as \( 1 + (-\ln y)^a \), where \( y \) is a random variable and \( a \) is an empirical parameter for controlling the random factor in the simulation. These two parameters range between \([0,1]\). Based on the preceding modules, the overall conversion probability of each land-use cell can be estimated using the following equation:

\[
TP_{x_i,y_i}^t = PG_{x_i} \times Q_{x_i,y_i}^t \times I_y^t \times R
\] (3)

where \( TP_{x_i,y_i}^t \) represents the combined probability of grid cell \( x_i \) to convert from the initial land-use labels to the target labels at the iteration time \( t \). \( PG_{x_i} \) represents the land-use development suitability of the cell \( x_i \) estimated by the CNN. \( Q_{x_i,y_i}^t \), \( I_y^t \), and \( R \) correspond to the neighborhood effects, inertia coefficient, and random factor, respectively. The overall conversion probability here is also in the form of a probability set (e.g. \( [TP_{x_i,y_1}^t \times TP_{x_i,y_2}^t \ldots TP_{x_i,y_m}^t] \)), representing the potential of each land-use label that may be allocated to the cell at time \( t \). The final mixed land-use allocations are determined by a multilabel learning threshold function (Yu, Pedrycz, and Miao 2014), which is defined as:

\[
y_{ij} = \begin{cases} 
1, & \text{if } TP_{x_i,y_j}^t \geq k \\
0, & \text{if } TP_{x_i,y_j}^t < k
\end{cases}
\] (4)

where \( k \) represents the threshold value and the cell is allocated to the specific land-use label (tagged as 1 according to the one-hot encoding) if the overall transition probability is greater than the threshold value; otherwise, the cell would not be allocated to the labels. Then, the optimized threshold value is determined to be:

\[
t = \arg\max_t (\text{sum}(\text{and}(y_i, y'_i)))
\] (5)

where \( y'_i \) is predicted label set and \( y_i \) is observed label set. The threshold value is between \([0,1]\). We can obtain the preliminary multi-label land-use simulation result with the optimized threshold. Furthermore, the conversion matrix, as a tool in expressing the conversion difficulty from the current land-use category to the target type, can contribute to a more realistic simulation result (Guan et al. 2011). Hence, according to the historical trend of land-use change in our study area, a conversion matrix was constructed based on the historical trend of land-use change. The final multi-label land-use allocation is determined through a continuous iterative simulation process. The iteration ends when total amount of labels for each land-use type reaches a target value (e.g. the total label amount of each land-use type of terminate year).

### 2.4. Accuracy assessment

Performance evaluation in multi-label learnings is much more complicated than in traditional single-label learnings, as each example can be associated with multiple labels simultaneously (Zhang and Zhou 2014). In this paper, we used the following methods for evaluating the performance and precision of the model. First, according to single-label learning, there are four measures to characterize the binary classification performance: TP (true positive), TN (true negative), FP (false positive), and FN (false negative). The sum of TP and TN is equal to the correct estimations, while the sum of FP and FN represents the unexpected and missing estimations. Based on the preceding definition, four overall evaluation metrics: Accuracy, Precision, Recall, and F1 are used for the assessment, which can be defined as follows:
\[ \text{Accuracy} = \frac{1}{N} \sum_{i=1}^{N} \frac{|y_i \cap y'_i|}{|y_i \cup y'_i|} \]  
(6)

\[ \text{Precision} = \frac{1}{N} \sum_{i=1}^{N} \frac{|y_i \cap y'_i|}{|y'_i|} \]  
(7)

\[ \text{Recall} = \frac{1}{N} \sum_{i=1}^{N} \frac{|y_i \cap y'_i|}{|y_i|} \]  
(8)

\[ F_1 = \frac{2 \cdot \text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}} = \frac{1}{N} \sum_{i=1}^{N} \frac{2|y_i \cap y'_i|}{|y_i| + |y'_i|} \]  
(9)

The other valid method of multi-label evaluation is Hamming loss, which can be defined as:

\[ \text{Hamming Loss} = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{m} |y'_i \Delta y_i| \]  
(10)

where \( \Delta \) represents the symmetric difference between two sets. The Hamming loss is defined for evaluating the fraction of misclassified instance-label pairs. Specifically, the larger values of the first four metrics correspond to the better results, while the Hamming loss has the opposite trend.

3. Study area and implementation

3.1 Study area

As one of the central cities of the Pearl River Delta (PRD) economic zone, Huizhou is administrated as a prefecture-level city with an area of 11,347 km\(^2\) and the inhabitants of approximately 4.8 million at the nominal year of 2019, according to the China national census. Specifically, the administrative division of the city includes two districts (Huicheng and Huiyang districts) and three counties (Huidong, Boluo, and Longmen counties), as shown in Figure 3. In recent
years, the city has promoted a convenient transportation network and the urban development zone to stimulate rapid urban development. With an increase of 6.16% population in the past 10 years and the accelerating economic growth, Huizhou is a representative city that involved rapid urbanization in China with large urban sprawl in the suburban area. However, due to the scarcity of land-use resources, the city is developing a compact urban structure with increasing density and complexity of land uses. Thus, under such a rapid urban growth circumstance, the city’s land-use dynamic could be more complex than before, leading to a great challenge for achieving sustainable urban development. Accordingly, to provide further insight into the mixed land-use evolution process of the city under such a rapid urbanization circumstance, we selected Huizhou city as a research region to simulate the mixed land-use change with the multi-label paradigm.

### 3.2 Data source and preprocessing

In this study, two main categories of data (i.e. land-use maps and a series of geospatial data) were used for model development. The original land-use vector data of Huizhou for 2009 and 2013 were obtained from the Chinese Academy of Sciences (CAS) ([http://www.resdc.cn/Dalist1.aspx?FieldTyepID=1,3](http://www.resdc.cn/Dalist1.aspx?FieldTyepID=1,3)), which involved 22 land-use classes in the raw maps. The land cover data in 2020 (WorldCover 10 m 2020) was collected from the European Space Agency ([https://esa-worldcover.org/en](https://esa-worldcover.org/en)). Then, we checked and corrected the misclassified land patches through visual interpretation based on the high-resolution Google satellite image and generated the multi-label land-use map. To simplify the maps for the multi-label modeling, we reclassified the original land-use maps into the four most representative land-use classes (see **Table 1**): agriculture, forest, urban, and other land, which can represent the main land-use types in our study area. Moreover, compared to the urban expansion, the change in water body area is relatively small in general. Thus, we excluded the water body in our modeling.

Specifically, multi-label land-use data are key to our modeling (i.e. each land-use grid cell can be allocated to multiple land-use types). This study used an effective algorithm to generate multi-label land-use maps based on original land-use vector data, which can be summarized as follows: (1) extracting the land-use vector map for each land-use type; (2) generating the raster land-use maps from the vector data with a specific resolution (i.e. 100 m in our study); and (3) aggregating all the raster maps to obtain the multi-label land-use maps. Hence, in this study, we generated the multi-label land-use map for Huizhou in 2009 and 2013 using the above approach (**Table 2**). Thereafter, the labels of all land-use grid cells were organized by one-hot encoding. Specifically, the one-hot encoding assigns labels in each cell as a set \( \{0,1\}^n \) (n indicates the land-use categories, which is four in this study). According to the land-use classification specified in **Table 1**, the labels in a set represent the land-use categories of “A”, “F”, “U”, and “O” respectively, where a label of 0 indicates that there is no specific land-use type within the cell (otherwise, 1). For example, a land-use cell of \([1, 0, 0, 0]\) indicates a pure agricultural land-use cell (i.e. “A”), while another cell of \([0, 0, 1, 1]\) represents a mixed land uses of urban and other land (i.e. “OU”). Such a practical and straightforward encoding approach has been widely adopted in multilabel learning to facilitate subsequent modeling processes. Based on the preprocessing, **Table 2** shows the multi-label land-use types and the label set in 2009, 2013, and 2020, respectively. The statistics suggest the accelerated urbanization and significant increase in land-use mixture and complexity of the city. For instance, the pure land-use cells of urban (U) and mixed cells of urban and other land (OU) have increased by 16.63% and 115.69% from 2009 to 2013, and by 94.20% and 60.28% from 2013 to 2020, correspondingly, suggesting a significant rapid growth of urban extent. In contrast, agriculture and forest land have decreased by 0.53% and 3.57% from 2009 to 2013.

### Table 1. Reclassification and labeling of land-use categories used in this study.

| Original land-use categories | Description                                                                 | Reclassed land-use Categories | Land-use label |
|-----------------------------|------------------------------------------------------------------------------|-------------------------------|----------------|
| Cropland                    | Land for growing crops                                                      | Agriculture                    | A              |
| Grassland                   | Grasslands growing mainly with herbaceous plants                            |                               |                |
| Woodland                    | Forestry land for growing trees, shrubs, bamboos, and coastal mangrove land | Forest                        | F              |
| Urban and rural settlement  | Urban built-up area and rural settlement                                     | Urban                         | U              |
| Other special land uses     | Other special land uses such as industrial and transportation land           | Other land                     | O              |
| Undeveloped land            | Land is not being used, such as bare land                                   |                               |                |

For instance, the pure land-use cells of urban (U) and mixed cells of urban and other land (OU) have increased by 16.63% and 115.69% from 2009 to 2013, and by 94.20% and 60.28% from 2013 to 2020, correspondingly, suggesting a significant rapid growth of urban extent. In contrast, agriculture and forest land have decreased by 0.53% and 3.57% from 2009 to 2013.
by 0.68% and 5.09% from 2013 to 2020. More specifically, the mixed land-use cells increased from 16.03% to 16.87% and to 17.00% of total land-use areas during the three stages. The mixture of land uses is likely to continue to increase in the future, as most mixed land-use units present a growing trend (e.g. the increase in mixed land-use cells for two consecutive time periods).

Previous studies have suggested that CA simulation correlates with various spatial variables, including environmental and socio-economic data (Chen et al. 2016; Liu et al. 2017; Verburg et al. 2002). These variables typically contain representative spatial information that drives the dynamics of land-use systems. Therefore, we collected a range of relevant driving factors for our model development, including transportation, topography, economy, and natural environment (shown in Table 3). These driving factors are preprocessed by minimum–maximum normalization and further adopted as inputs for the VGG-based network to further derive mixed land-use development suitability. We preprocessed all the driving factors and the multi-label land-use maps by projecting to the WGS84 coordinate system and setting to a uniform spatial resolution of 100 m with 1696 rows and 1643 columns (see Figure 4).

### 3.3. Model implementation

According to our designed framework, the ML-CNN-CA mainly involves two modules: the VGG-based network and the modified multi-label CA model. To evaluate the performance of the proposed model, we applied the model to the Huizhou city with rich spatial data for multi-label land-use change simulation of 2009, 2013, and 2020. For the VGG-based network, we adopted a stratified sampling strategy based on the multi-label land-use category (as shown in Table 2) to select representative samples for training and validation, where 60% of the samples (~660,000 cells) are selected for training and 40% (~443,282 cells) were used for validation and feedback. This strategy can ensure that each land-use label in CNN modeling have representative samples. For the CA module, a series of parameters in the submodules (i.e. neighborhood effect, self-adaptive inertia coefficient, and the random factors) were calibrated and optimized using the CA calibration procedure. Based on the preliminary calibration of the model, a 3 × 3 optimal neighborhood size, threshold value of 0.55, and other optimal parameters were specified for the model simulation. Furthermore, we examined various settings that are sensitive to the performance of the model in the calibration procedure, such as the window size for calculating the neighborhood effect and the conversion control matrix (in Section 4.3).

As the final control step of the model, the label-level-based conversion matrix is shown in Table 4, which indicates the conversion rules of each land-use label within a cell. Specifically, we mainly assume that the urban and other land are not allowed to convert to agriculture and forest land, whereas other land-use label conversions are all allowed. Thus, a land-use cell that has already developed label of “U” or “O” is impossible to be degraded in the following iterations. The simulation continues to iterate until all land-use changes reach the macro-demand of each land-use type at the terminated year. In addition, given the

Table 2. Observed multilabel land-use category statistics in 2009, 2013, and 2020.

| Category | Label set | Land-use cells in 2009 | Land-use cells in 2013 | Land-use change rate between 2009–2013 | Land-use cell in 2020 | Land-use change rate between 2013–2020 |
|----------|-----------|------------------------|-----------------------|-----------------------------------------|----------------------|----------------------------------------|
| A        | [1, 0, 0, 0] | 204,318                | 203,238               | −0.53%                                  | 201,858              | −0.68%                                  |
| F        | [0, 1, 0, 0] | 672,944                | 648,937               | −3.57%                                  | 615,882              | −5.09%                                  |
| U        | [0, 1, 0, 0] | 35,824                 | 41,782                | 16.63%                                  | 81,139               | 94.20%                                  |
| AFO      | [0, 0, 0, 1] | 17,394                 | 27,223                | 56.51%                                  | 20,963               | 23.00%                                  |
| AFU      | [1, 1, 0, 0] | 113,538                | 105,688               | −6.91%                                  | 78,065               | −26.14%                                  |
| AU       | [1, 0, 1, 0] | 19,529                 | 20,246                | 3.67%                                   | 19,261               | −4.87%                                  |
| AO       | [1, 0, 0, 1] | 9,418                  | 15,950                | 69.36%                                  | 32,674               | 104.85%                                 |
| FU       | [0, 1, 1, 0] | 16,274                 | 15,973                | −1.85%                                  | 9,836                | −38.42%                                 |
| FO       | [0, 1, 0, 1] | 11,184                 | 14,980                | 33.94%                                  | 24,476               | 63.39%                                  |
| LIO      | [0, 1, 1, 1] | 3,218                  | 6,941                 | 115.69%                                 | 11,125               | 60.28%                                  |
| AFU      | [1, 1, 1, 0] | 1,963                  | 2,836                 | 44.47%                                  | 2,171                | −23.45%                                 |
| AFO      | [1, 0, 1, 0] | 1,407                  | 2,617                 | 86.00%                                  | 7,413                | 183.26%                                 |
| AOU      | [1, 0, 1, 1] | 741                    | 1,079                 | 45.61%                                  | 2,023                | 87.49%                                  |
| FOU      | [0, 1, 1, 1] | 423                    | 643                   | 52.01%                                  | 1,172                | 82.27%                                  |
| AFUO     | [1, 1, 1, 1] | 30                     | 72                    | 140.00%                                 | 147                 | 104.17%                                  |
stochastic perturbation of the random factor, the final accuracies (including the model comparison) were averaged and the simulation maps were determined through repeated tests to ensure robustness of results. The final simulated results were required to ensure that each cell was assigned to the same individual land-use label with over 90% in the repeated experiments. The proposed ML-CNN-CA model was implemented using Python 3.9 with the Scikit-learn (https://scikit-learn.org/stable/) and Numpy (https://numpy.org/) packages, and the CNN module in our research was developed based on TensorFlow (https://www.tensorflow.org/) and Keras (https://keras.io/) tools.

4. Results

4.1. Calibration and Validation of VGG-based network

Here we designed two experiments to validate the VGG-based network performance respectively on (1) the comparison on different CNN architectures and (2) the evaluation of the VGG-based network on each multi-label land-use type. We adopted three representative deep learning architectures to benchmark the CNN performance, including the GoogleNet (Szegedy et al. 2015), ResNet (He et al. 2016), and AlexNet (Krizhevsky, Sutskever, and Hinton 2017) for comparison. For all the networks, the number of epochs is 100, the learning rate is 1e-4 and decay be 0.1, Adam optimizer is adopted and beta1 is 0.9. And all the CNN architectures are modified based on our input one-dimensional spatial data. Table 5 shows the overall comparison results of four CNN architectures (i.e. VGG-, GoogleNet-, ResNet-, and AlexNet-based network) based on multiple quantitative measurements in a micro averaging. We find that the VGG-, GoogleNet- and AlexNet-based architectures present a satisfactory performance in multi-label land-use simulation tasks (i.e. precision and AUC measurements are over 0.84 and 0.94, respectively), while the VGG-based achieves the best accuracy of all measurements (precision = 0.853, recall = 0.782, f1 = 0.816, AUC = 0.951). This result may be significantly related to the data structure of the adopted spatial factors, which needs further examination on different datasets. In summary, the VGG-based model can achieve satisfactory performance in excavating spatial factors to derive multi-label land-use suitability.

In addition, we adopted the receiver operating characteristic (ROC) curves and the area under the ROC curve (AUC) values (Fawcett 2006) (see Figure 5) to illustrate the performance of the proposed VGG-based network on each multi-label land-use type. Here, given the ROC curve illustrating the diagnostic ability of the binary classifier, we derived the curves based on the four land-use categories. Moreover, overall ROC curves for multilabel tasks are derived based on macro- and micro-average methods.

### Table 3. Spatial driving factors used in this study.

| Index | Driving factors     | Resolution/ data                     | Data resource                                      | Year | Categories               |
|-------|---------------------|--------------------------------------|----------------------------------------------------|------|--------------------------|
| 1     | DEM                 | ~30 m                                | SRTM Digital Elevation Model                       | 2000 | Natural factors          |
| 2     | Slope               | ~30 m                                | Derived from DEM                                    | 2000 |                           |
| 3     | Distance to water   | 100 m                                | Derived from original land-use vector data         | 2009 |                           |
| 4     | Distance to urban   | vector                               | OpenStreetMap                                       | 2010 | Location factors         |
| 5     | Distance to district center | vector | OpenStreetMap                                      | 2010 |                           |
| 6     | GDP                 | ~1 km                                | Gridded global datasets for Gross Domestic Product and Human Development Index | 2010 | Socio-economic factors   |
| 7     | Population          | ~1 km                                | The Gridded Population of World Version 4 (GPWv4)  | 2010 |                           |
| 8     | Distance to main road | vector | OpenStreetMap                                      | 2010 | Transportation factors   |
| 9     | Distance to railway | vector                               | OpenStreetMap                                       | 2010 |                           |
| 10    | Distance to highway | vector                               | OpenStreetMap                                       | 2010 |                           |
| 11    | Distance to traffic junction | vector | Gaode Map Services                                 | 2010 |                           |
| 12    | Distance to bus station | vector | Gaode Map Services                                 | 2010 |                           |
Specifically, the macro-average method calculates the metrics for each label and finds their unweighted mean, whereas the micro-average method calculates metrics globally by considering each element of the label indicator matrix as a label. A larger area under the ROC curve suggests a better model performance, and the AUC value varies between 0 and 1, where 1 represents perfect fitting performance. Figure 5 shows the ROC curves and AUC values of all land-use types and the overall evaluation. Specifically, the overall macro- and micro-average AUC values are 0.904 and 0.951,
respectively. Result suggests that the VGG-based network achieves satisfactory fitting performance for each land-use category through the collected driving factors as the AUC values of each land-use type are exceeded 0.85, especially the AUC values of forest and urban are over 0.9. Overall, the VGG-based network has demonstrated the feasibility of using the collected driving factors to derive land-use suitability for simulation.

Based on the well-trained VGG-based network, Figure 6 further shows the spatial patterns of land-use suitability for four land-use categories, which provide spatial details to understand how the spatial patterns of land-use evolution were developed in the simulation. In this study, each cell contains four development suitability values corresponding to the land-use types; therefore, the higher the probability, the more likely the land-use label could be allocated. Generated by the VGG-based network, the development suitability maps suggested a high-probability aggregation with urban areas (Figure 6) and other lands (Figure 6) in the central and southern parts. Forest and agriculture (Figure 6) are more likely to be found at the city’s periphery (i.e. northeastern part for agriculture land and northwestern part for forest land).

### 4.2. Simulation results and model comparison

By integrating land-use suitability, neighborhood effects, self-adaptive inertia coefficient, stochastic factor, and conversion constraints, we first calibrated the proposed model based on 2009 and 2013 and further stimulated the multi-label land-use change from 2013 to 2020 for accuracy assessment. Figure 7 presents a confusion matrix based on each land-use label (shown in Table 2) for the previous (2009–2013) and latter (2013–2020) periods. Overall, the matrixes show the high consistency between the simulation results and the actual mixed land-use patterns as the overall accuracy (OA) and Kappa coefficient are 88.98% and 0.81 for 2009 to 2013, and 84.04% and 0.75 for 2013 to 2020, correspondingly. In particular, the mixed land-use units with two categories present a good agreement with reality for both 2013 and 2020 (i.e. the percentages of simulated as positive are mainly over 50%), which suggests that the proposed model is practical for capturing complex mixed land-use evolution. However, we discover that mixed land-use cells with complex labels have limited simulation accuracy according to the matrixes. The complex competitions and interactions between these land-use units and their surrounding land, which may be difficult to model with general transition rules, are largely responsible for this result.

In addition, Table 6 further shows a binary evaluation of each land-use label for the simulated and observed multi-label land-use data both for 2013 and 2020. The classification measures between simulated and observed map are shown as the total labels’ percentages. Result reveals that the multi-label land-use simulation results among agriculture, forest, and urban land reach high accuracy with precision, recall, and F1 measures all exceeding 0.84 for 2013, and 0.74 for 2020. However, the other land-type simulation results have relatively low accuracy according to the three measures. There are two main possible reasons for this result. First, this study's category of other land reclassified is highly complex interior, which government planning policies may significantly influence. Thus, this land-use type can be difficult to model through general CA transition rules. Moreover, samples of other land are relatively less than the sample of the other three types for training, suggesting a great challenge in capturing the dynamic land-use change. This unbalanced sampling in multi-label classification tasks is common, so mapping the relationship between explanatory variables and labels could be a major challenge for categories with fewer samples (Liu, Blekas, and Tsoumakas 2022). Therefore, it is possible to further improve the simulation results by incorporating a variety of urban planning factors (Liang et al. 2020).

| Table 4. Label-level-based land-use conversion matrix (1 = conversion possible; 0 = conversion not possible). |
|---|---|---|---|---|
| Label convert to | A | F | U | O |
| A | 1 | 1 | 1 | 1 |
| F | 1 | 1 | 1 | 1 |
| U | 0 | 0 | 1 | 0 |
| O | 0 | 0 | 1 | 1 |

| Table 5. Overall assessments on different convolutional neural network architectures. |
|---|---|---|---|
| Network | Precision | Recall | F1 | AUC |
| GoogleNet | 0.851 | 0.765 | 0.806 | 0.946 |
| ResNet | 0.721 | 0.618 | 0.665 | 0.845 |
| AlexNet | 0.845 | 0.787 | 0.815 | 0.949 |
| VGG-based Net | 0.853 | 0.782 | 0.816 | 0.951 |
Figure 8 presents the actual multi-label land-use patterns of 2009 and 2013, and the simulated results of 2013, while Figure 9 shows the actual and simulated multi-label land-use patterns of 2020. The global simulated pattern showed high spatial consistency with the actual land uses across the city. Results also indicate that the simulated spatial details of multi-label land-use change can agree well with actual mixed land-use patterns. Furthermore, we also found a significant urban sprawl and increased land-use mixture during the study periods in Figures 8 and 9, which corresponds to the land-use statistic in Table 2. The visualization of the simulation results (see Figures 8 and 9) reveals that the majority of urban land developed in the city’s central and southern areas, which primarily clustered in the Huicheng (i.e. the political center of the city) and Huiyang districts (i.e. the main economic development zones of the city). Furthermore, cropland was primarily distributed around urban land, while woodland was located outside of the study area. Also, we can see the transitional development of mixed land uses. In other words, mixed land uses are more likely to develop at the intersection of multiple land-use types. For example, in the city’s suburban area, the pure cropland cell with label could gradually change to mixed cropland and urban land cell with label due to rapid urbanization.
To examine the effectiveness of the deep-mining strategy and interactive mechanism of our model, we compared the ML-CNN-CA model with another multi-label land-use change model (ML-CA-LTM) (Ormani 2017) in the same study area. Specifically, the ML-CA-LTM model is a CA-based model that adopts an artificial neural network (ANN) algorithm with backpropagation (BP) multilabel learning to derive the overall CA conversion probability. The model has been proven to be practical for simulating mixed land-use dynamics under the multi-label concept. Here, Table 7 shows the comparison results of the simulation performance between the ML-CNN-CA model and the ANN-based ML-CA-LTM model for 2013 and 2020. According to all quantitative measurements, the proposed model performs better on the multi-label land-use change simulation. The model achieves the best performance for overall evaluation (accuracy = 0.912, hamming loss = 0.048) in the calibration process (i.e. results for 2013), while the simulation result for 2020 is acceptable (accuracy = 0.896, hamming loss = 0.055). More specifically, the ML-CNN-CA model surpasses the previous model by 5.80% and 10.89% of accuracy, 2.97% and 9.67% of precision, 5.17% and 9.81% of recall, and 4.94% and 10.71% of f1 for 2013 and 2020, respectively. This result demonstrates the effectiveness of our proposed model for mining mixed land-use change transition rules.

Moreover, to further investigate the model performance on mixed land-use dynamics, we assessed the simulation results focused on mixed land-use grid cells (i.e. land-use cells if more than two categories). Compared to the previous model, the simulation results of the proposed model show significant improvement in capturing the mixed land-use change...
than the previous model (accuracy = 0.658 and 0.618; hamming loss 0.191 and 0.208) both for 2013 and 2020 (i.e. improved by 0.17 and 0.09 for accuracy, and 0.09 and 0.05 for hamming loss). These results suggest that integrating deep-mining strategy and interactive mechanism in mining the CA transition rules can help better simulate the complex mixed land-use evolution, which are the major improvements in our proposed model.

4.3. Sensitivity analysis

Given that different settings in the CA calibration have shown significant influences on the simulation results (Pan et al. 2010; Shafizadeh-Moghadam et al. 2017), we tested two main parameters of the models (i.e. the neighborhood size and the conversion matrix) based on the model calibration of 2009 and 2013. The neighborhood window size is an essential setting for calculating the neighborhood interaction rules, affecting the overall land-use conversion of CA. This study implemented the ML-CNN-CA model and tested the Moore neighborhood of sizes $3 \times 3$, $5 \times 5$, and $7 \times 7$ to verify the sensitivity of spatial filters by controlling other experimental conditions. As shown in Table 8, the simulation accuracy gradually decreased as the window size increased, as the average accuracies of the model were 0.912, 0.871, and 0.811, with Hamming losses of 0.048, 0.069, and 0.106 for neighborhood sizes of $3 \times 3$, $5 \times 5$, and $7 \times 7$, respectively. Moreover, Figure 10 illustrates the spatial error maps based on different window sizes, further demonstrating that a $3 \times 3$ window size achieves better performance for the simulation. This result suggests that a smaller window size in the neighborhood effect achieves a better mixed land-use change simulation result based on our proposed model. This result could mainly be attributed to the smaller window size, allowing more adjacent details to be modeled within the neighborhood effects. Thus, the small window size of $3 \times 3$ in our model is more capable of mining the transition rules for mixed land-use dynamics.

The conversion matrix is another module that may affect the model performance. According to Figure 11, compared to the results without the conversion control, the multi-label land-use spatial patterns are more similar to the observed spatial distributions under the control of the

laws according to all measurements. We found that the proposed model can achieve satisfactory results on mixed land-use cells with higher accuracy (0.823 and 0.711) and lower hamming loss (0.098 and 0.158)
conversion matrix. The Accuracy, Precision, Recall, and F1 of the simulation results based on the conversion matrix are improved by 2.36%, 4.00%, 13.06%, and 7.23%, respectively, compared to the results that allow all the conversions (i.e. sample model without the conversion matrix).

Overall, according to the calibration of our model, a smaller neighborhood window, and
a control conversion matrix can help the model perform more realistic mixed land-use simulations.

4.4. Importance of spatial driving factors

Identifying the contributions of each driving factor in the land-use change modeling can help urban planners further understand how these factors drive or matter land-use evolution (Feng and Tong 2017; Lv et al. 2021), which is crucial for developing appropriate and effective land-use planning policies (Zhang et al. 2019). This study adopted a specific CNN network to derive mixed land-use suitability based on multiple collected driving factors. In contrast to the interpretable models (e.g. linear regression or Tree-based models), which are scalable and permit easy computation of the importance of variables, neural network-based methods are generally difficult to derive the feature explanations due to their intrinsic black-box nature. However, SHapley Additive exPlanations (SHAP) is an effective method to explain individual predictions for neural network-based approaches by computing the contribution of each feature to the model (Lundberg and Lee 2017). Also, the SHAP value could provide global and local interpretability for overall feature explanations and each observation explanation, which significantly increases the transparency of neural network-based models.

Here, we measured the factor importance by deriving the overall SHAP values (i.e. the averaged absolute SHAP values of observations) of all the driving factors based on each land-use category. Figure 12 shows the rank of average SHAP values for the four land-use categories. Overall, the natural factors are more valuable for agriculture and forest land modeling in our study, whereas the socio-economic and transportation factors play a more crucial role in urban and other land simulations. Specifically, DEM is the most valuable factor for

Figure 9. Simulated multi-label land-use pattern and details of 2020. (a) Actual multi-label land-use map in 2020. (c) Simulated multi-label land-use map in 2020.
Table 7. Comparison of simulation results for two CA-based models under multi-label concept (ML-CNN-CA/ ML-CA-LTM).

| Model                          | Accuracy | Precision | Recall | F1      | Hamming loss |
|-------------------------------|----------|-----------|--------|---------|--------------|
| Overall evaluation            | ML-CNN-CA| 0.912     | 0.937  | 0.935   | 0.934        | 0.048         |
|                               | ML-CA-LTM| 0.862     | 0.910  | 0.889   | 0.890        | 0.069         |
| Mixed land-use evaluation     | ML-CNN-CA| 0.823     | 0.903  | 0.893   | 0.874        | 0.098         |
|                               | ML-CA-LTM| 0.658     | 0.894  | 0.674   | 0.740        | 0.191         |

Table 8. Evaluations on different neighborhood sizes of the proposed model.

| Size   | Accuracy | Precision | Recall | F1   | Hamming loss |
|--------|----------|-----------|--------|------|--------------|
| 3 × 3  | 0.912    | 0.937     | 0.935  | 0.934| 0.048        |
| 5 × 5  | 0.871    | 0.887     | 0.927  | 0.894| 0.069        |
| 7 × 7  | 0.811    | 0.775     | 0.925  | 0.851| 0.106        |

agriculture and forest land as indicated by the SHAP values of 6.23% and 5.33%, respectively, followed by the slope (i.e. SHAP value of 4.66% for agriculture land and 3.99% for forest land). Population (2.05%) and GDP (1.48%) factors contribute the most to urban land simulation, and the GDP (1.98%) and distance to bus station (1.12%) factors are most significant for the other lands modeling. Generally, agriculture and forest land evolutions are mainly influenced by the natural environment, such as elevation conditions and water resources; thus, natural drivers show the greatest contribution to these two land-use changes. In contrast, urban and other lands, as the central area of urban activity, their dynamics are largely determined by human activities and planning policies (Liang et al. 2020; Yao et al. 2017). The feature explanation results provide supplementary information to understand the contribution of each driver based on the proposed VGG-based network, which shows great potential in helping decision-makers and planners to develop urban management policies.

5. Discussion

Given the increased intensity and diversity of urban space to date, simulating the mixed land-use evolution is useful for planners and policymakers to understand the mixed land-use structure and interactions, and thereby support the allocation of scarce land resources toward sustainable urban development (Abdullahi and Pradhan, 2018). To this end, this study developed a multi-label CA model (ML-CNN-CA) to investigate the mixed land-use changes with the multi-label learning strategy and modified multi-label CA transition rules. In the proposed model, each CA grid cell was labeled by multiple land-use types rather than a single land-use type in traditional CA models, which enabled the model to simulate mixed land-use changes in urban areas. Our practice of applying the ML-CNN-CA model in a fast-developing city has shown the proposed model’s effectiveness for the mixed land-use change simulation as it achieves satisfactory simulation performance (examined based on quantitative accuracy assessment in Figure 7 and Tables 6 and 7 and morphological inspections in Figures 8 and 9).

Based on existing studies, only a few explorations have focused on studying the mixed land-use change. A multi-label strategy is one of the direct manners to formalize the mixed land uses by assigning multiple land-use types to each grid cell. In this study, we also adopted the multi-label strategy for mixed land-use modeling. Our practices demonstrated that the multi-label concept could integrate different intelligent mechanisms for the modeling with wide expandability for different applications. Furthermore, the multi-label strategy can reduce the complexity of capturing multi-dimensional interaction rules of mixed land-use dynamics. Unfortunately, the interaction of mixed land-use change have been simplified in previous CA models, leading to difficulties in performing more realistic simulation under current accelerated urban mixed land-use development (Liang et al. 2021; Omrani, Tayyebi, and Pijanowski 2017). Here we adopted a deep-mining strategy (i.e. a specific CNN architecture) and three interactive mechanisms (i.e. the neighborhood effect, adaptive inertia coefficient, and random factor) implemented under the multi-
Figure 10. Error maps of four land categories based on different neighborhood sizes.

Figure 11. Comparison of the spatial patterns for the results based on allowing all conversions and based on conversion matrix.
The label concept to overcome the above limitations. These modules were tightly integrated to mine the complex interaction rules of mixed land-use change and proved to have good performance and significant improvement compared to the previous model. Relevant experimental results also demonstrate the effectiveness of our adopted modules, such as the CNN architecture comparison (Table 5 and Figure 5) and the sensitivity analyses (Table 8 and Figures 10 and 11). Also, the modeling framework can be improved by coupling diverse mechanisms to be adopted for different study areas or urban applications.

As we have examined the sensitivity of our adopted submodules, results indicate that the simulation performance can be influenced by different model or parameter settings. These settings will need to be examined through the CA calibration process when applied to other regions, which are the crucial factors that affect the simulation performance for different case studies (Santé et al. 2010). In addition, understanding the importance of spatial drivers is essential to enable the practicability of the mixed land-use simulation model for urban management. Here we used a SHAP method to quantitatively measure their importance (Figure 12). The results vary for applications in different regions, and it also requires further examinations to further generalize the proposed model for other regions and time periods.

Overall, the mixed land-use evolution is a complex human-nature dynamic interaction process. It can be influenced by multidisciplinary factors such as planning, government policy, environmental effects and human activities. The proposed model still needs further examinations for different regions to show its practicability, which has not been tested in this study due to the time and data costs. Nevertheless, the CA-based models usually have specific paradigms and definitions to enable it can be applied to various local areas through the model calibration process (Berberoğlu, Akin, and Clarke 2016; He et al. 2018; Kafy et al. 2021; Qian et al. 2020) or global scale (Chen et al. 2020; Li et al. 2017). Similar to other CA-based models, our modeling methodology has clear paradigms and definitions, which hopefully can be applied to different regions for simulating urban mixed land-use change with relevant spatial data.

6. Conclusion

Previous studies have not sufficiently investigated mixed-use changes and their evolution as the land grid cell is usually simplified as one single land-use type. This study mainly explores the methodological framework to simulate mixed land-use changes by developing a ML-CNN-CA model with the multi-label learning strategy. We applied and examined
the proposed ML-CNN-CA model in Huizhou, a fast-developing city in the Guangdong-Hong Kong-Macao Greater Bay Area of change, to simulate the mixed land-use changes during 2009–2013 and 2013–2020. Results demonstrate that the ML-CNN-CA model achieves satisfactory simulation performance (i.e. accuracy = 0.912 and 0.896, hamming loss = 0.048 and 0.055, for 2009–2013 and 2013–2020, respectively) and good morphological patterns against actual land-use changes. The model comparison results also show significant outperformance of the proposed model against the previous ANN-based multi-label CA (ML-LTM-CA) model. In summary, the proposed model is examined to be effective in mining the complex interaction rules of mixed land-use change, indicating its capability in simulating mixed land-use change for the city. Moreover, the proposed model still needs further examinations for different regions or applications to evaluate its sensitivity and show wide applicability. The practice of this study can serve as a guide to model and simulate mixed land-use change under the current accelerated development of urban complex and compact land-use structures, thus showing great potential in achieving sustainable urban development.

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Data and codes availability statement

The data and codes that support the findings of this study are available at figshare.com (10.6084/m9.figshare.14762838).

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