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RESEARCH ARTICLE

A new cellular automata framework of urban growth modeling by incorporating statistical and heuristic methods

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ABSTRACT

We develop a new geographical cellular automata (CA) modeling framework, named UrbanCA, through reconstructing the essential CA structure and incorporating nonspatial, spatial, and heuristic approaches. The new UrbanCA is featured by 1) the improvement of the CA modeling framework by reformulating relationships among CA components, 2) the development of two scaling parameters to adjust the effects of transition probability and neighborhood, 3) the incorporation of a variety of statistical and heuristic methods to construct transition rules, and 4) the inclusion of urban planning regulations and spatial heterogeneities to project future urban scenarios. To illustrate the effectiveness of UrbanCA, we calibrate a CA model using artificial bee colony (ABC) to simulate the past urban patterns and predict future scenarios in Shanghai of China. The results show that UrbanCA under different scaling parameters is comparable to CA-Markov (as a reference model) concerning the accuracy of the end-state and change simulations, and is better than CA-Markov regarding the driving factor's ability to explain the modeling outcomes. UrbanCA provides more choices compared to existing CA software packages, and the models are readily calibrated elsewhere to simulate the dynamic urban growth and assess the resulting natural and socioeconomic impacts.

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UrbanCA; urban growth modeling; statistical method; heuristic algorithm; scaling parameter

1. Introduction

Exploring spatiotemporal urban growth, understanding land use dynamics, and evaluating the influence of long-term land use change are frontier scientific issues of concern in the international geographical information sciences (GIS) and geography communities (Huang *et al*. 2009, Mitchell *et al*. 2018, Song *et al*. 2018, Huang *et al*. 2019). Geographical simulation using GeoComputation and cellular automata (CA) is an effective approach to understanding the dynamic spatial processes (Li *et al*. 2013, Ghisu *et al*. 2015, Clarke 2019) as well as to optimizing the spatial planning and allocation of land use (Newland *et al*. 2018a, Tong and Feng 2019). CA modeling has become a standard method for simulating complex systems (Crooks 2016) because of its bottom-up mechanism to reproduce the systems driven by underlying interactions (Xia *et al*. 2019). While geographical CA modeling can capture past changes and predict future scenarios and has

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achieved great progresses so far (Hasan *et al*. 2017), it still faces challenges such as the improvement of primary methods, the retrieval of transition rules, the objective parameterization for multi-scenario prediction, the integration of multiple methods, and the improvement of simulation accuracy. To address these crucial issues adequately, we developed a new spatial modeling tool for dynamic urban growth by incorporating statistical and heuristic methods.

Geographical CA modeling originated in the 1970s when Tobler applied cell-based models to simulate Detroit's rapid urban expansion (Clarke 2018b). Tobler was the first to note that the core feature of CA models is the inclusion of neighborhoods, i.e. the local geographical factors. After White and Engelen (1993) used CA models to simulate the urban land use evolution, they became popular in urban and land use studies. Following the rapid development of remote sensing, GIS, and spatial analysis technologies, many CA modeling software packages have emerged (Basse *et al*. 2016, Liu *et al*. 2017, Pinto *et al*. 2017, Feng and Tong 2018a). These played an important role in understanding the Earth's surface changes and addressing human-land relationships in the contexts of population explosion, rapid economic growth, and global warming (Whitsed and Smallbone 2017, Newland *et al*. 2018b).

Examples of geographical CA modeling developments include UrbanSim, DUEM, Dinamica EGO, SLEUTH, CLUE-S, SIMLANDER, APoLUS, FLUS, GeoSOS, SPRAWL, and CA-Markov. UrbanSim is an operational urban simulation model (Waddell 2002) to manage the side effects of urban expansion and residential location. Dinamica EGO is a software platform that implements multi-transitions to analyze and simulate space-time phenomena (Ferreira *et al*. 2019). SLEUTH is a popular CA-based urban growth modeling tool that incorporates influencing factors including slope, land use, exclusion, urban extent, transportation and hill shade (Clarke *et al*. 2018a). CLUE-S models the changes of multiple land use types in a raster-based space by combining the top-down allocation of land use change and the bottom-up land use transition rules (Verburg *et al*. 2002, Kucsicsa *et al*. 2019). SIMLANDER and APoLUS are two packages of land use modeling for the R environment, allowing the dynamic interaction of neighborhood, accessibility, suitability and zoning (Hewitt *et al*. 2018). FLUS integrates a system dynamic model and a CA model to simulate multiple LUCC scenarios by coupling human and natural effects (Liu *et al*. 2017, Chen *et al*. 2019). This tool also incorporates planning policies to project future urban growth scenarios and delineate their boundaries for evaluating the potential outcome of the present policies (Liang *et al*. 2018). GeoSOS is a software package of geographical simulation and optimization by integrating CA, agent models, and swarm intelligence (Li *et al*. 2011). SPRAWL is a recently developed stochastic urban growth model to predict alternative scenarios (Mcgarigal *et al*. 2018). CA-Markov is an integrated model of CA and Markov Chain, and is included in IDRISI for land allocation and land cover prediction (Aburas *et al*. 2017). Among the modeling tools, SLEUTH and CA-Markov may be the most popular modeling packages (Onsted and Clarke 2012, Saxena and Jat 2018, Wu *et al*. 2019, Xu *et al*. 2019). While the tools differ in their framework, structure and algorithms, they all can be used to simulate urban growth and project future scenarios.

Despite progress in CA modeling, challenges remain in urban growth mapping, modeling and learning (Pontius *et al*. 2018). Among these, key modeling challenges include model calibration and validation, model errors and uncertainties analysis, model repeatability, model comparison and scale effect analysis (Thill and Dragicevic 2018). In terms of model construction and calibration, two important issues must be addressed:

(1) In a typical CA model, fundamental components such as the cell transition probability, the neighborhood effect, the constraints, and the stochastic factor are multiplied to convey cell state information in processing (García *et al*. 2013, Liao *et al*. 2016, Mirbagheri and Alimohammadi 2017, Feng and Tong 2018b). This kind of information transmission is somehow problematic because the overall transition probability cannot exceed a predefined threshold and the state change will stop no matter how many iterations are implemented, if the probability is small enough. As a consequence, it is insufficient to address the spatial complexity of land use dynamics. Specifically, in such typical CA models, a cell must satisfy both the transition probability and the neighborhood effect to change its state. This means that a cell cannot change its state if the transition probability is high but the neighborhood effect is weak, or if the transition probability is low but the neighborhood effect is strong. In practice, actual land transitions often occur when only one of these conditions is met, that is, as long as one of these values (the transition probability and the neighborhood effect) is higher than a threshold, the cell likely changes its state.
(2) In simulation, cells with higher probabilities have greater opportunities to be transformed from nonurban to urban and the remaining persistent cells usually relate to lower probabilities, suggesting the decreasing effect of transition probability over time; meanwhile, the locations near urban cells may attract more nonurban-to-urban transformations despite of the decreasing effect of transition probability, suggesting the increasing effect of neighborhood over time. In extreme, the transition probability may become sufficiently small and the potential nonurban-to-urban transformation can only be attributed to the neighborhood effect. A typical CA model does not try to eliminate such side effects, leading to the loss of dispersedly distributed land patches and the increase in strongly aggregated landscape patterns as compared to the true land use (urban) patterns. These departures can be substantial when there is a long time interval (e.g. ~20 years or more) between the start-to-end period of model calibration.

The above issues show that temporally persistent transition probability and neighborhood effect cannot express the spatiotemporal land use dynamics to generate accurate simulations. Therefore, it is necessary to improve the CA model structure and develop new software to provide more solutions for urban growth simulation, hence supporting the estimation of the natural and socioeconomic impacts of future urban development. Here, we propose an improved CA modeling framework that addresses the modeling challenges by incorporating adjustable parameters, land use regulation layers, and landscape heterogeneity maps. We then develop a new UrbanCA tool of urban growth modeling, which is freely available for modelers. To construct CA models for different case studies, UrbanCA incorporates nonspatial and spatial statistical methods to retrieve land transition rules and three categories of heuristics to optimize land transition rules. A new CA model and the UrbanCA tool were tested with a case study at Shanghai, a rapidly urbanizing area of China. Our approach improves the simulation accuracy in urban growth modeling, provides reliable predictions of multiple urban scenarios, and offers accurate simulations of spatial processes of large-scale environmental phenomena.

2. Urbanca: a new CA modeling framework

2.1 The modeling framework

The UrbanCA tool has four parts: basic technique architecture, transition rule modeling, model implementation, and model assessment (Figure 1). UrbanCA extends existing studies by introducing the probability scaling and neighborhood scaling into the primary CA approach as well as by incorporating actual urban planning regulation and spatial heterogeneity into the model implementation. UrbanCA's graphical user interface (GUI) has five menus: spatial data reading, statistical method, heuristic algorithm, model run, and validation (Figure 2).

- **Basic technique architecture**: UrbanCA is constructed using the ArcGIS interfaces of spatial data processing, R packages of statistical and heuristic methods, and

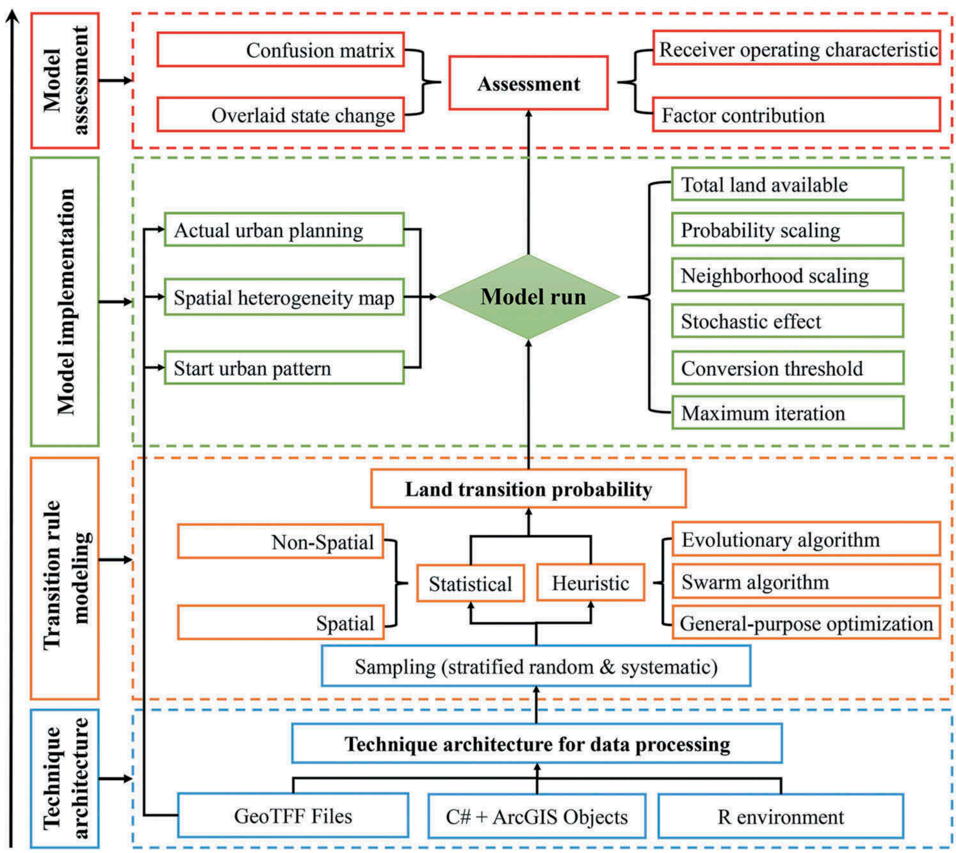

Figure 1. The UrbanCA architecture for modeling dynamic urban growth.

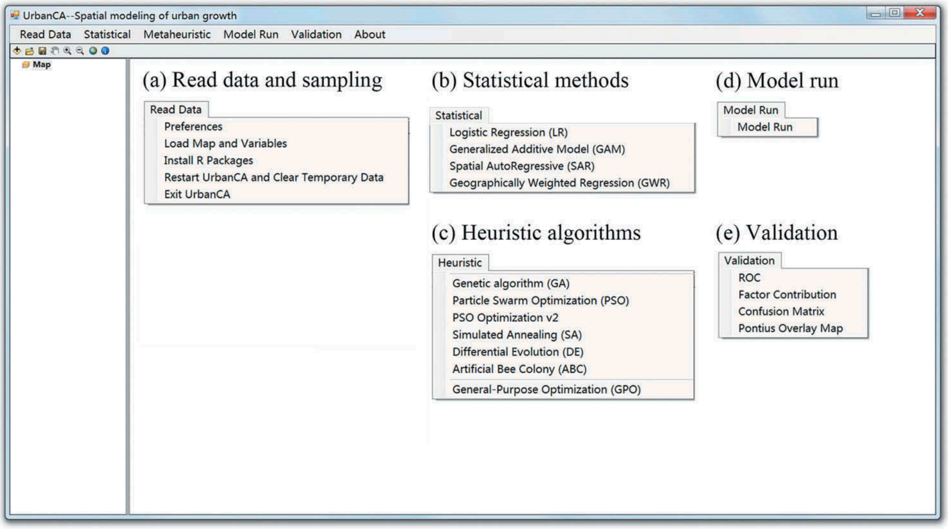

Figure 2. The UrbanCA's GUI showing data input, transition rule modeling, model run, and model assessment.

input map layers in a generic Geo-TIFF format. The integration of these techniques can sufficiently process the nonspatial and spatial datasets for CA modeling.

- **Transition rule modeling**: Samples for model training can be selected using stratified random sampling and systematic sampling. A number of statistical methods and heuristic algorithms are incorporated into UrbanCA to generate land transition probability maps.
- **Model implementation**: UrbanCA can simulate past-to-present urban patterns and project future scenarios by defining land transition probability, neighborhood effect, stochastic effect and constraints. It also considers the impacts of urban planning regulation and spatial heterogeneity in the landscape.
- **Model assessment**: Four model assessment methods are included in UrbanCA to evaluate the land transition probability, the factors' explanatory ability to the simulated outcomes, the simulated end-state, and the simulated change.

2.1.1 An improved urban modeling framework

In a typical CA model, the state of each cell at a specific time step is defined by a transition function that considers the combined effects of the cell state at the previous time step, the land transition probability, the neighborhood effect, the nonspatial and spatial constraints, and the related stochastic perturbations (García *et al*. 2013, Munshi *et al*. 2014). The transition function can be represented as (White and Engelen 1993, Wu 2002):

$$State \cdot Next = TranFunc(State \cdot Present, P_{conv}, NeiConfig, Res, RND)_i \qquad (1)$$

where *TranFunc* denotes the transition function with states including urban, nonurban and water body; *State·Present* and *State·Next* denote the cell state at the present time step and the next time step, respectively; P_{conv} denotes the temporally static land transition probability calculated using driving factors; *NeiConfig* denotes the neighborhood effect that represents the bottom interactions among nearby cells; *Res* denotes both the nonspatial constraints that consider the total land available for development and the spatial constraints that inhibit cell state transition at a specific location; and *RND* denotes a stochastic factor that simulates the unknown perturbations leading to the mutation of cell state.

In UrbanCA, we propose an improved modeling framework by improving the primary formula of a typical CA model as follows:

(1) We use union (sum) instead of intersection (product) to reflect the combined effects of transition probability and neighborhood influence. The union suggests that, as long as the transition probability or neighborhood influence exceeds the threshold, the cell being processed can change its state at the next time step.
(2) We introduce a time-increment parameter (TIP) to resist the decaying effect of transition probability. The TIP scaling can adjust the transition probability according to the aim of specific studies, resulting in effective representation of the factor's influence on urban growth.
(3) We introduce a local adjustment parameter (LAP) to reduce the abnormal influences caused by the increasing neighborhood effect during the model simulation. The LAP scaling can result in the accurate transmission of the bottom interactions among nearby cells.

Here, both TIP and LAP are scaling parameters to adjust the effects of CA components. With these three improvements, the transition function in UrbanCA can be given by:

$$\begin{cases} P_{all} = (P_{conv} \times (1 + S_{TIP})^{t-1} + P_{ni,t} \times S_{LAP} \times S_{HET}) \times M_{PLAN} \times Res \times Rnd/2 \\ \qquad s.t.\ spatial\ and\ nonspatial\ constraints \end{cases} \tag{2}$$

where P_{all} is the overall transition probability a cell transforming from nonurban to urban; S_{TIP} is a TIP ranging between 0.0 and 0.1 where 0.0 denotes no incremental effect and 0.1 denotes a high incremental effect; S_{LAP} is a LAP ranging between 0.5 and 1.0 where 0.5 denotes a moderate neighborhood effect and 1.0 denotes a full neighborhood effect; S_{HET} is landscape heterogeneity reflecting the unevenness and complexity of urban growth; and M_{PLAN} is actual planning regulation on urban development. The optimal TIP and LAP are defined using a trial-and-error experiment by searching for the highest simulation accuracy. We provide the UrbanCA default settings with TIP 0.01 and LAP 0.8, which are defined by extensive pre-experiments.

2.1.2 Modeling land transition probability

Modeling land transition probability is a key step in geographical system simulation. The core issue is the definition of the best factorial combination and the retrieval of CA parameters. Many methods have been applied to define the transition rule for mapping land transition probability. Among the representative techniques that can build transition rules are statistical and heuristic methods. The major difference is that the statistical methods directly regress the samples to estimate the CA parameters, whereas the heuristics automatically search for the parameters to fit the samples. For both approaches, the land transition probability can be calculated as (Wu and Webster 1998, Munshi *et al*. 2014, Jafari *et al*. 2016):

$$P_{conv}(a) = \frac{\exp(\boldsymbol{a}\cdot\boldsymbol{x} + by + \varepsilon))}{1 + \exp(\boldsymbol{a}\cdot\boldsymbol{x} + by + \varepsilon)} = \frac{\exp(a_0 + a_1x_1 + \ldots + a_ix_i + \ldots + a_nx_n + by + \varepsilon))}{1 + \exp(a_0 + a_1x_1 + \ldots + a_ix_i + \ldots + a_nx_n + by + \varepsilon)} \quad (3)$$

where $\boldsymbol{a} = (a_0, a_1, \ldots, a_n)$ are the CA parameters of urban growth factors [independent variables x_i (i = 0,1, ..., n) with x_0 = 1], b is the weight of the dependent variable (y) if an autoregressive model is applied to the transition probability, and ε is the modeling residual.

(1) *Statistical methods* (Table 1) incorporated in UrbanCA include *nonspatial* techniques such as logistic regression (LR) and generalized additive model (GAM), and *locally spatial regression* techniques such as spatial autoregressive (SAR) and geographically weighted regression (GWR). To produce accurate predictions of dependent variables, nonspatial regression minimizes the sum of the squares of the predicted residuals while spatial regression eliminates the spatial clusters and autocorrelation of the residuals. Figure 3 shows examples of GUIs of SAR and GWR for producing land transition probability maps, where these tools were developed using the R packages *spdep* and *lctools*, respectively.
(2) *Heuristics* are optimization algorithms to calibrate CA transition rules (García *et al*. 2013, Whitsed and Smallbone 2017). Such algorithms search for near-optimal parameters by minimizing the residuals (Feng and Tong 2018a) that can be evaluated by the root-mean-square error (RMSE), relative error (RE), and mean absolute error (MAE). Based on these metrics, we constructed the standard forms of objective functions for heuristic algorithms in CA modeling. They are given by:

$$\begin{cases} Method1 \rightarrow RMSE : Minimize\ F_1(\boldsymbol{a}) = \sqrt{\frac{\sum_i^m (P_{conv}(\boldsymbol{a}) - Act_o)_i^2}{m}} \\ Method2 \rightarrow RE : Minimize\ F_2(\boldsymbol{a}) = \frac{\sum_i^m |P_{conv}(\boldsymbol{a}) - Act_o|_i}{\sum_i^m Act_{o,i}} \\ Method3 \rightarrow \mathrm{MAE} : Minimize\ F_3(\boldsymbol{a}) = \frac{\sum_i^m |P_{conv}(\boldsymbol{a}) - Act_o|_i}{m} \\ \qquad \text{s.t. Bounds and inequality of parameters} \end{cases} \quad (4)$$

where $F_{1-3}(\boldsymbol{a})$ are the objective functions, $P_{conv}(\boldsymbol{a})$ is the predicted transition probability,

Table 1. The nonspatial and spatial statistical methods used in UrbanCA.

Category	Method
Nonspatial	*Logistic regression* (LR) fits samples where the dependent variable is binary such as urban and nonurban (WU 2002). *Generalized additive model* (GAM) fits samples through flexible smooth functions and ranks the driving factors according to their explanatory deviance.
Spatial	*Spatial autoregressive* (SAR) considers the spatial autocorrelation (local Moran's I) among selected samples in retrieving CA transition rules. *Geographically weighted regression* (GWR) incorporates spatial heterogeneity into spatially non-stationary CA transition rules where each driving factor contains effects that both promote and resist urban growth.

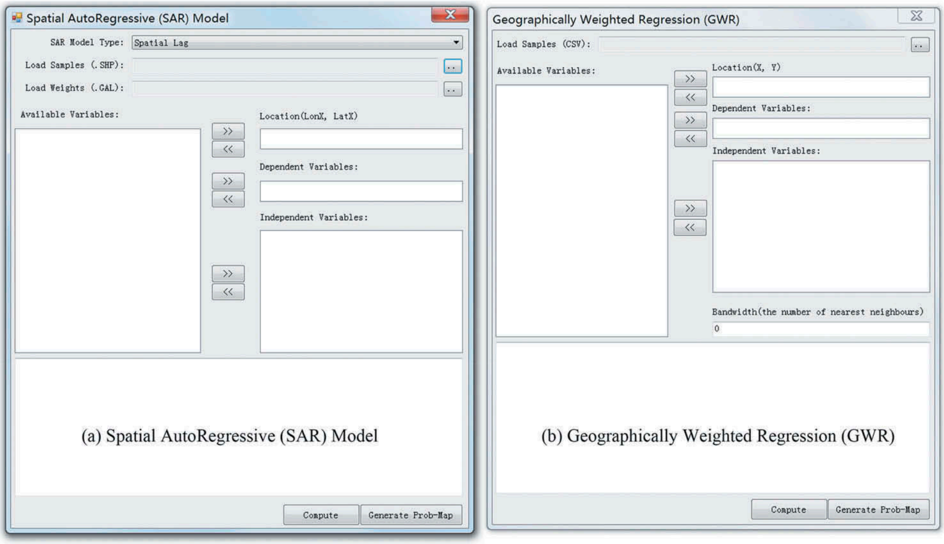

Figure 3. GUIs for SAR and GWR to generate land transition rules and probability map.

Act_o is the observed urban growth, m is the number of selected samples, (lower and upper) bounds are the ranges for all parameters, and inequality is an additional constraint for the parameters.

The objective functions can be categorized as either differentiable or non-differentiable. They are the information sources for heuristic optimization in searching for the extrema. For CA-based urban growth modeling, the residual based objective functions are discrete and not differentiable, and therefore cannot be solved using classical statistical methods. Table 2 lists three categories of heuristics that are included in UrbanCA to generate land transition probability maps. All these heuristics have been proven successful to integrate with CA

Table 2. Heuristic algorithms incorporated into the UrbanCA framework.

Category	Algorithm
Evolutionary algorithm	Evolutionary algorithms (EAs) are generic population-based heuristics inspired by biological evolution, which commonly incorporates selection, crossover and mutation operators. EAs can be applied to resolve the extrema of differentiable and non-differentiable functions. Among the EAs, *genetic algorithm* (GA) and its variants are the most widely applied methods in calibrating CA models (JENERETTE and WU 2001, García *et al*. 2013). Recently, *differential evolution* (DE) has also been used to calibrate CA models to simulate past and future land use patterns (FENG and TONG 2018a).
Swarm algorithm	Swarm intelligence (SI) algorithms relate to a cluster of heuristics developed by modeling the behaviors of different swarming animals and insects (KARABOGA and AKAY 2009). Among the SI algorithms, *particle swarm optimization* (PSO) and *artificial bee colony* (ABC) have been widely applied in optimizing CA parameters to generate more accurate land transition probability, hence more accurate simulation outcomes (NAGHIBI *et al*. 2016).
General-purpose optimization	General-purpose optimization is another category of heuristics to search for the minimum of non-linear objective functions with bound constraints. These include widely applied generalized *simulated annealing* (SA) and many other methods in the R package '*optimx*'. The *optimx* consists of *Nelder-Mead* (NM), *Broyden-Fletcher-Goldfarb-Shanno* (*BFGS*), *Limited-memory BFGS* (L-BFGS-B), *spectral projection gradient* (SPG), *conjugate gradient* (CG), and *non-local mean* (NLM), and so on.

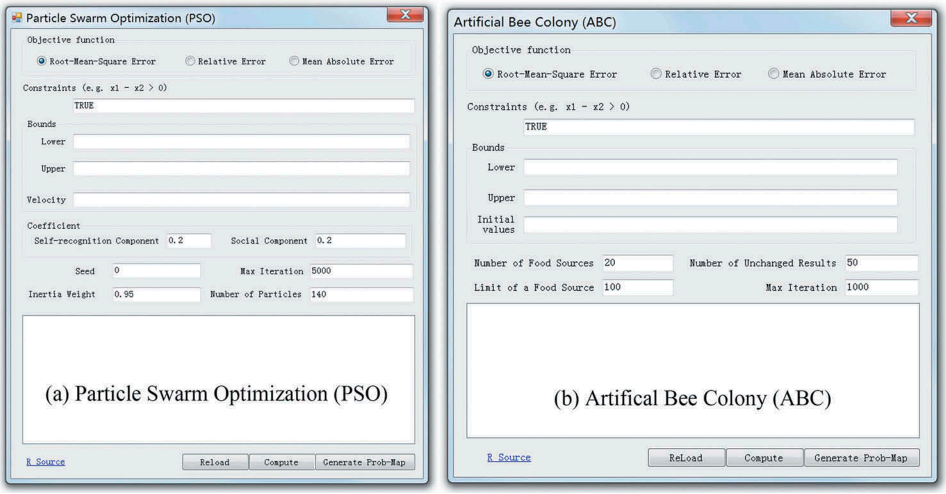

Figure 4. GUIs of two selected heuristics to generate land transition rules and probability map.

models of land use change and urban growth (Cao *et al*. 2011, García *et al*. 2013, Liao *et al*. 2016, Mcgarigal *et al*. 2018). Figure 4 shows examples of GUIs for two heuristics that can be readily applied to capture CA transition rules and then to generate the land transition probability maps. UrbanCA also provides a web link in each GUI that directs the modelers to the corresponding R source. In addition, other popular methods such as support vector machine, ant colony optimization and neural networks are under development and will be incorporated in UrbanCA soon.

2.1.3 Neighborhood configuration

Neighborhood effect [$P_{ni,t}$ in Equ.(2)] is a unique CA component that features a 'bottom-up' approach. The neighborhood configuration reflects how CA models self-organize to produce complex systems (Wu *et al*. 2012). Tessellation-based CA models can incorporate regular and irregular neighborhood, while vector-based CA models incorporate only irregular neighboring patches. Conventional CA models contain fundamental principles of homogeneous cellular systems (Codd 2014), but urban growth is spatially non-stationary or heterogeneous. As a result, the homogeneous neighborhood configuration cannot accurately capture the spatial heterogeneity in land use and urban growth (Feng and Tong 2019), leading to larger simulation errors. We provide three configuration options that include regular neighborhood, irregular neighborhood, and spatial heterogeneity weighted neighborhood to sufficiently address the urban growth dynamics:

(1) *Regular neighborhood* is common in CA models (Jenerette and Wu 2001, Wu *et al*. 2012). It includes rectangle, circle, annulus and wedge, where a square with the same width and height (*e.g.* 5 × 5 square neighborhood) is most widely applied.
(2) *Irregular neighborhood* can reflect complex urban growth dynamics, and has been applied in a number of publications (Dahal and Chow 2015, Barreira-González and Barros 2017). Before implementation, an irregular kernel is defined to address the

neighborhood shape and the weight of neighboring cells. For details, modelers can refer to the ESRI manual of focal-statistics.

(3) *Spatial heterogeneity weighted neighborhood* (SHWN) is realized by overlaying a map of spatial heterogeneity in urban land use change (Feng and Tong 2019). In the SHWN configuration, nonurban cells have unequal opportunities for development and the spatial heterogeneity can be applied to both the regular and irregular neighborhoods.

2.1.4 Global and local constraints

Constraints [*Res* in Equ.(2)] are crucial factors in simulation as they measure impediments to the nonurban-to-urban land conversion under certain conditions. In the literature, the total land available for development is the global constraint serving as the model termination criterion (White *et al*. 1997). Local constraints are employed to restrict urban cells being allocated in predefined areas such as broad water bodies, ecologically protected areas, and basic farmlands. In addition to global and local constraints, CA models sometimes include urban planning constraints to identify areas that can only be partially developed.

2.1.5 Stochastic effects

Stochastic effects [*RND* in Equ.(2)] in CA models are used to simulate unknown disturbances in urban growth (White and Engelen 1993, Feng and Tong 2018a). The stochasticity may be caused by policy changes, the modification of urban regulations, and/or the failure to implement urban plans. For example, to maximize developer economic benefit, new apartments are often inserted into a large area of farmland far from urban public infrastructure such as subways, trains and major roads. UrbanCA simulates these uncertainties using a stochastic factor with a self-memory random seed throughout the modeling procedure. The use of memorable seeds ensures the robustness of CA modeling because the simulations of the same case implemented at different times do not change substantially.

2.1.6 The overall transition rule and threshold

Integrating all these components into Euq.(2), UrbanCA calculates the overall transition probability (P_{all}) and produces transition rules for CA implementation. In the decision rule, if P_{all} is larger than a predefined threshold, a nonurban cell outside the constrained areas will become an urban cell; otherwise, the nonurban cell retains its current state. In UrbanCA, the threshold is defined using a trial-and-error approach based on the given number of iterations and the total land available for development. The number of iterations is usually defined as multiples of the year from the start map to the final map used to calibrate the CA models. The model terminates when the sum of simulated urban cells reaches the total land cells available for development. The implementation GUI in the UrbanCA framework is shown in Figure 5. The planning map for spatial constraints, the spatial heterogeneity map for neighborhood effect, and the stochastic factor are optional items for the model run. TIP and LAP are implemented in the modeling run GUI and are respectively named as neighborhood scaling and probability scaling.

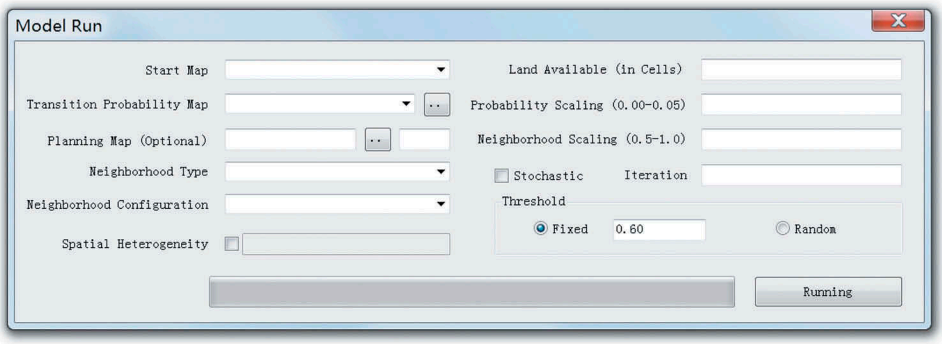

Figure 5. The GUI of UrbanCA model run.

2.2 Assessment and validation

2.2.1 End-state assessment

We include an error matrix in UrbanCA to assess the end-state of simulations. The matrix calculates the cross-tabulated areas through a cell-by-cell comparison between the simulated urban pattern and the actual urban pattern, and reports overall accuracy, average accuracy (producer's accuracy), average reliability (user's accuracy), commission error, and omission error. The error matrix also reports false positives, false negatives, true positives, and true negatives to generate a ROC curve. According to PONTIUS and Millones (2011), a few other metrics can also be derived from the error matrix. These include Kappa coefficient and its variants, quantity agreement and disagreement, and allocation agreement and disagreement.

To compare the landscape patterns of the simulated and predicted results, we calculate several landscape metrics including number of patches (NP), largest patch index (LPI), edge density (ED), largest shape index (LSI), mean patch area (AREA_MN), perimeter-area fractal dimension (PAFRAC), and mean Euclidean nearest-neighbor distance (ENN_MN). The landscape similarity of urban patterns between the BAU-scenario and a different scenario can be calculated by:

$$LS = \left(1 - \frac{\sum abs\left(\frac{M_{scenario} - M_{bau}}{M_{bau}}\right)}{n}\right) \times 100\% \tag{5}$$

where LS is the landscape similarity, M_{bau} is a landscape metric of the BAU-scenario, M_{scenario} is the same landscape metric of another scenario, and n is the number of landscape metrics.

2.2.2 Change assessment

Earlier studies also suggest the change assessment by overlaying the starting reference urban pattern, the final reference urban pattern, and the final simulated urban pattern (Pontius *et al*. 2011, Liu *et al*. 2014). For urban growth simulation, the overlay generates five categories: Urban at the initial time, Hit growth, Missed growth, Falsely allocated growth, and Correctly rejected nonurban persistence. Hit growth signals that reference urban growth was correctly simulated as growth in the model. Missed growth signals that reference urban growth was incorrectly rejected as nonurban persistence. Falsely allocated growth signals that reference nonurban persistence was incorrectly simulated as growth. The overlay map not only provides spatial visualization of accuracy and error, but also provides a quantitative assessment that can be transformed to those derived from an error matrix. By considering Hit growth, Missed growth, and Falsely allocated growth comprehensively, the Figure of Merit (FOM) can be calculated to indicate the percentage of Hit among the sum of the actual and simulated changes. Moreover, a variant of Kappa, named Ksimulation, was included to evaluate the agreement between the simulated and actual urban growth (Van Vliet *et al*. 2011).

2.2.3 Factor contribution

We present a new method based on GAM to assess the factor contribution to the simulation results. It offers a quantitative explanation of driving factors for the simulated past/current urban patterns and the predicted future scenarios. GAM detects the non-linear relationships between the modeled changes by nonparametric smoothing functions, hence explores the importance of factors using modeling deviance. A standard GAM can be given by (Hastie 2017):

$$LC(u) = b_0 + S_1(x_1) + \ldots + S_i(x_i) + \quad \ldots \quad + S_k(x_n) \tag{6}$$

where $LC(u)$ is a link function, b_0 is the intercept (constant), $S_i(x_i)$ is a smoothing function that links $LC(u)$ and the driving factors (x_i), and n is the number of driving factors.

There is no substantial difference between the GAM for building CA models and the one used here. For CA model construction, the GAM captures the relationships between the past urban growth and its driving factors to define CA transition rules; whereas, for factor contribution explanation, the GAM examines the relationships between the simulation results and their factors to assess the simulation reliability. In model assessment, the rank-order of driving factors is determined by the modeling residual deviance where a factor with larger deviance has higher importance. The contribution of all factors can be given by:

$$PDE = \frac{MD.NULL - MD.ALL}{MD.NULL} \times 100\% \tag{7}$$

where *PDE* is the percentage deviance (i.e. factor contribution) explained by all factors, *MD.NULL* is the deviance when there are no factors, and *MD.ALL* is the deviance when inputting all factors.

3. Application and case studies

3.1 Study areas and datasets

To test the usability, ability, and predictive power of UrbanCA, we applied a CA model based on an artificial bee colony method (ABC-CA) to simulate the urban growth at Shanghai of China, and then compared the UrbanCA results with those from CA-Markov in IDRISI. Shanghai is economically central of China and consists of 16 districts covering 6,340 km^2 (Figure 6). The city has experienced very rapid urban expansion as

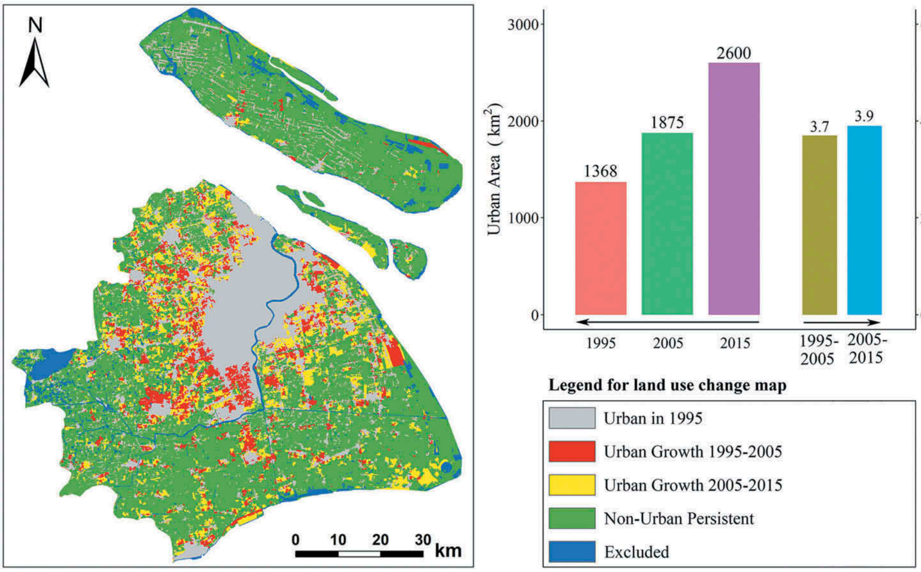

Figure 6. Dynamic urban growth at Shanghai during 1995–2015.

demonstrated by its annual urban growth rate (~3.8%) and has doubled its urban area from 1,368 km^2 in 1995 to 2,600 km^2 in 2015. In the last decade, Shanghai has been selected as an ideal place for studies to examine various aspects related to urban issues (Feng and Tong 2017, Huang *et al*. 2019).

3.2 Transition rules and maps

To build the ABC-CA models, we selected urban growth driving factors that reflect spatial proximity to facilities, terrain conditions, population, and economy. These are the distances to city centers (CITY), district centers (DIST), road networks (ROAD) and subway (SUBW), digital elevation model (DEM), population density (POP), and gross domestic product (GDP). We used these factors as independent variables, and used 1995–2005 urban growth as the dependent variable.

We trained the transition rules using ABC and calibrated the ABC-CA models with 4,953 sample points selected by systematic sampling. The ABC-CA models were applied to simulate the 2005 and 2015 urban patterns and predict future scenarios out to the year 2025. In this study, we have four future scenarios: 1) Business-as-usual (BAU) scenario that assumes the continuation of current trend; 2) DIST-scenario that emphasizes the effects of district centers; 3) ROAD-scenario that emphasizes the effects of road networks; and 4) POP-scenario that emphasizes the effects of population distribution. In practice, BAU-scenario transition rules were retrieved based on the objective function with no constraints, while the transition rules of the other three scenarios were retrieved based on the objective function with specific constraints where the absolute value of the emphasized factor is greater than the other factors. These constraints are represented as

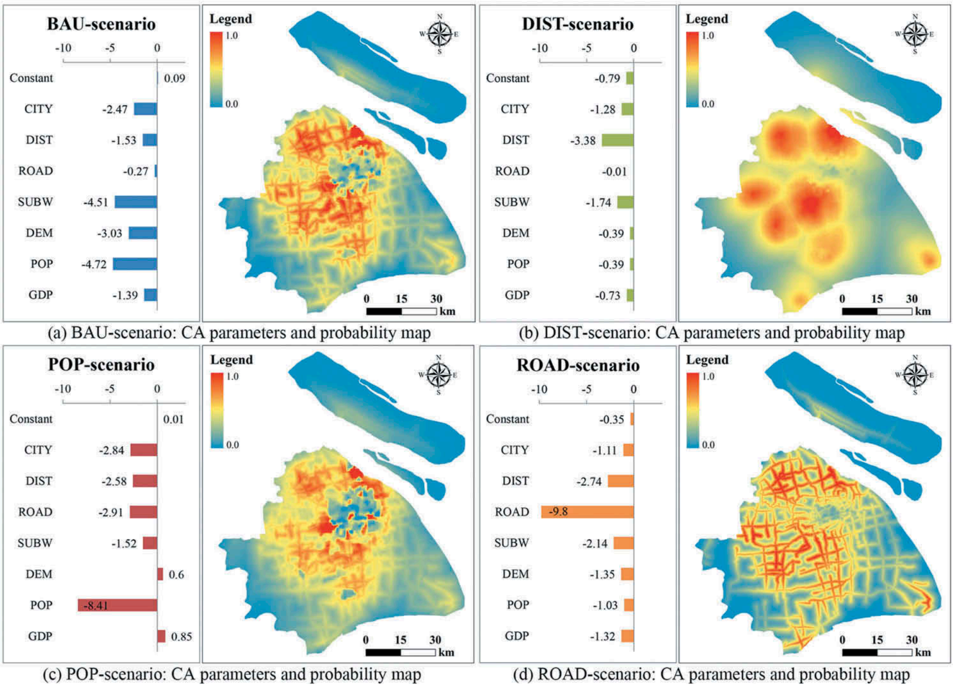

Figure 7. CA parameters of transition rules and the corresponding land transition probability maps.

inequalities attached to the objective function. For example, the inequality in Equ.(4) for the DIST-scenario was represented as:

$$\begin{cases} |DIST| > |ROAD|, and|DIST| > |ROAD|, and|DIST| > |SUBW|, and \\ |DIST| > |DEM|, and|DIST| > |POP|, and|DIST| > |GDP| \end{cases} \quad (8)$$

where CA parameters were computed under these constraints, which indicate the strongest impact of the DIST factor.

Figure 7 shows the CA parameters retrieved using ABC and the corresponding land transition probability maps. For the BAU-scenario, subway and population density are the two most influential factors; for other scenarios, each probability map was characterized by the emphasized factor. The parameters and maps show great differences between each other, implying substantial differences between the projected scenarios.

3.3 Simulation results and assessment

Each running parameter in Figure 5 was defined before model implementation. In this study, the planning map was not applied because our tests did not involve planning regulations, but readers can refer to Tong and Feng (2019) for detail if their studies need to examine the effects of actual urban planning. The neighborhood type was a square and the configuration was an extended 5 × 5 grid. Spatial heterogeneity map was produced using the gradient of land use patterns by following Feng and Tong (2019). The total land available was assigned the actual urban quantity for the 2005 and 2015

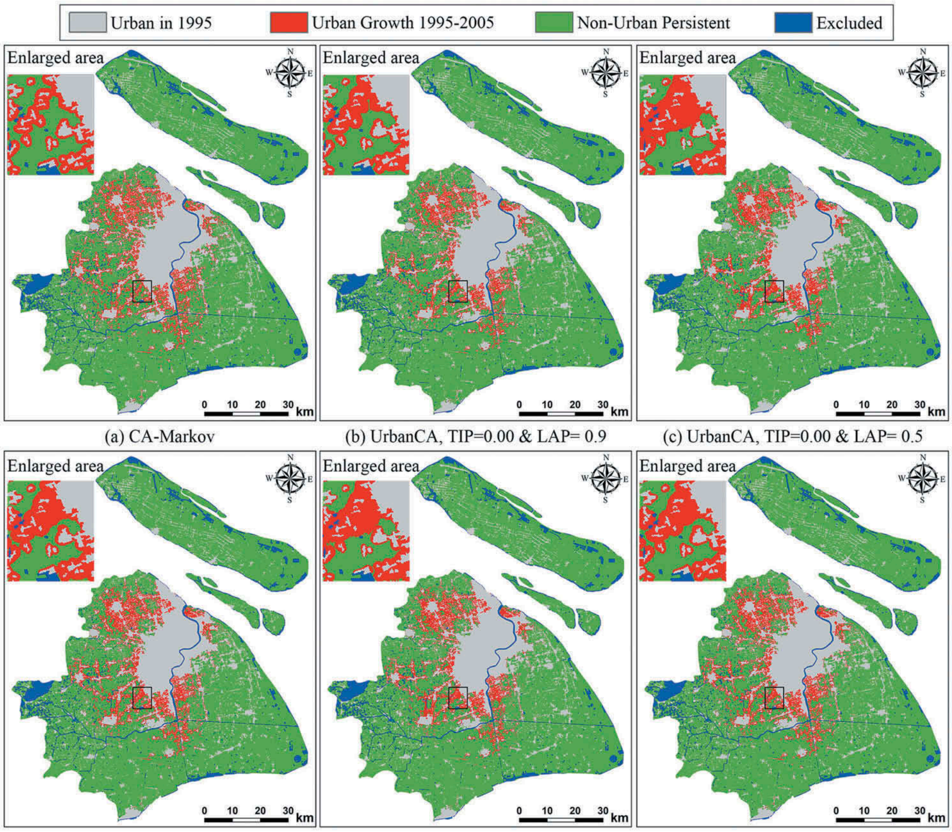

Figure 8. Modeling dynamic urban pattern in 2005 using CA-Markov and UrbanCA.

simulations; whereas, this was defined using a Markov chain for the 2025 predictions. To test the impacts of the probability scaling and neighborhood scaling, we applied five sets of parameters to the UrbanCA implementation. Each iteration represented one year and the fixed threshold was in the interval of 0.3 and 0.4; consequently, each implementation corresponded to a different threshold to generate the most accurate results at the maximum iterations.

Figure 8 shows that the 1995–2005 urban growth mainly occurred in the nearest regions surrounding the 1995 urban areas. Visually, there is high similarity between all the 2005

Table 3. Assessment of end-state and urban change for the 2005 simulations.

			End-state (%)	Change (%)						Landscape	
Model	TIP	LAP	Overall accuracy	Hit	Miss	False	FOM	$K_{simulation}$	PDE (%)	AREA_MN	PAFRAC
Actual										74.63	1.42
CA-Markov	N/A	N/A	89.4	2.5	5.3	5.3	19.1	24.7	18.6	91.05	1.41
	0.00	0.9	90.0	2.3	5.5	4.4	18.7	24.6	19.2	83.26	1.40
	0.00	0.5	90.1	2.2	5.5	4.3	18.5	24.4	21.8	80.94	1.43
UrbanCA	0.05	0.8	90.0	2.3	6.9	4.5	18.8	25.2	21.1	88.08	1.41
	0.02	0.8	89.6	2.5	5.3	5.0	19.4	24.7	21.0	79.00	1.32
	0.01	0.8	89.6	2.5	5.3	5.1	19.4	25.2	20.5	89.00	1.40

simulations and the actual pattern, and high similarity between the simulations from CA-Markov and UrbanCA under different scaling parameters. The similarity is confirmed by the overall accuracies greater than 89% for CA-Markov and UrbanCA (Table 3). However, the end-state assessment cannot adequately indicate the modeling ability of the models. The change assessment can better indicate the models' ability, which shows the scaling parameters substantially affect the change assessment metrics and factor contribution. Among all scaling parameters, TIP 0.01 and LAP 0.8 correspond to the highest FOM (19.4%), the highest Ksimulation (25.2%), and a moderate factor contribution (20.5%). In comparison, CA-Markov has the lowest overall accuracy (89.4%), a moderate FOM (19.1%), a moderate Ksimulation (24.7%), and the lowest factor contribution (18.6%). The landscape metrics show that the simulations have greater mean patch area (AREA_MN) than the observation where CA-Markov produced urban pattern yielding the highest mean patch area; in contrast, the shape complexity (PAFRAC) of all urban patterns has no substantial differences. While CA-Markov and UrbanCA appear to have similar simulation ability regarding the accuracy, CA-Markov yields weaker factor contribution that is surpassed by the UrbanCA with the most suitable scaling parameters.

We then used the ABC-CA models to predict the 2015 urban patterns (Figure 9), which also show high similarity between the simulated and observed, and between CA-Markov

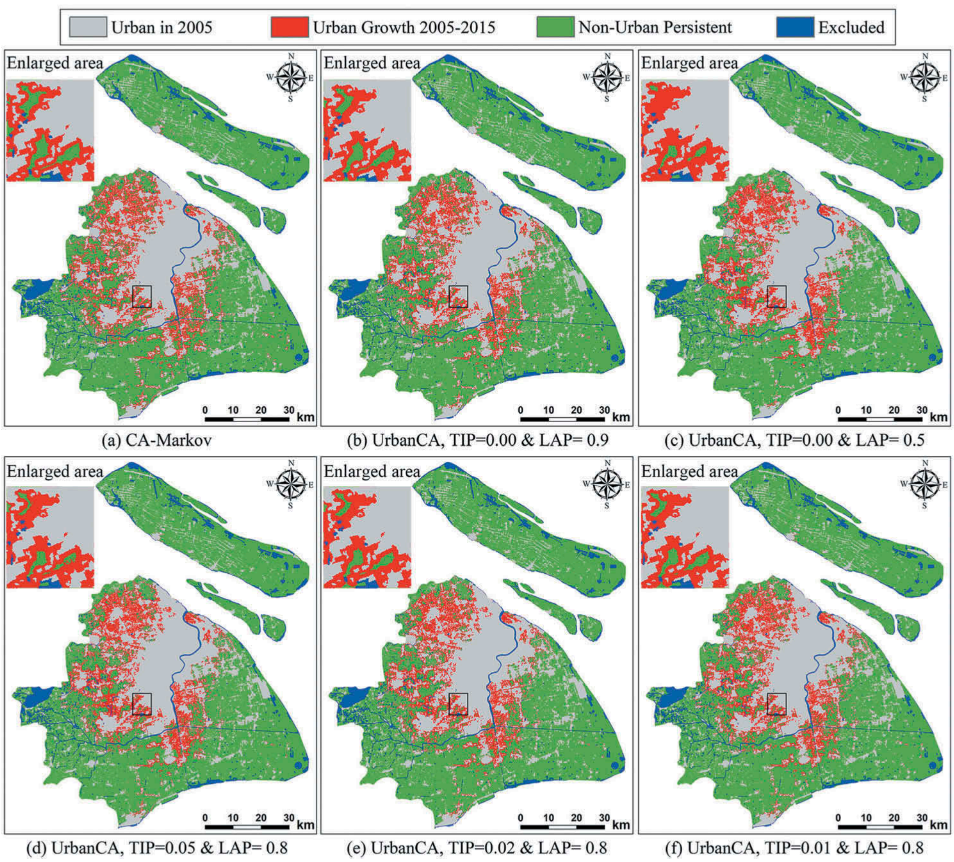

Figure 9. Modeling dynamic urban pattern in 2015 using CA-Markov and UrbanCA.

Table 4. Assessment of end-state and urban change for the 2015 simulations.

			End-state (%)	Change (%)						Landscape	
Model	TIP	LAP	Overall accuracy	Hit	Miss	False	FOM	$K_{simulation}$	PDE (%)	AREA_MN	PAFRAC
Actual										131.43	1.41
CA-Markov	N/A	N/A	86.8	4.5	6.6	6.6	25.4	29.6	19.6	157.44	1.35
	0.00	0.9	86.7	4.3	6.8	6.0	25.2	29.6	20.3	146.09	1.34
	0.00	0.5	86.9	4.2	6.9	6.1	24.6	28.8	24.4	142.69	1.37
UrbanCA	0.05	0.8	86.9	4.4	6.7	6.4	25.2	29.4	23.9	139.77	1.28
	0.02	0.8	87.0	4.4	6.7	6.3	25.3	29.7	22.3	147.87	1.35
	0.01	0.8	86.9	4.5	6.6	6.5	25.6	29.8	21.7	152.01	1.33

and UrbanCA. The built-up area in the city center continued to expand during 2005–2015. All overall accuracies exceed 86% and there are no substantial differences among them (Table 4). UrbanCA with TIP 0.01 and LAP 0.08 has the highest FOM and that with TIP 0.00 and LAP 0.5 has the lowest FOM, with CA-Markov generating FOM between them. Ksimulation that describes the simulation change indicates similar performance as FOM. Among all modeling schemes, the factors explain the most change generated by UrbanCA with TIP 0.00 and LAP 0.5 but the smallest change by CA-Markov. Compared to the 2005 simulations, the 2015 simulations have lower overall accuracies by ~3%, but higher FOM by ~6%, Ksimulation by ~5%, and PDE by ~2%. The landscape metrics show that, similar to 2005, the 2015 simulations have bigger mean patch area (AREA_MN) than the 2015 observation where the CA-Markov yielded the highest differences with the observation; whereas, the shape complexities (PAFRAC) of all simulations are slightly lower than the observation. The validation shows that 1) the two scaling parameters substantially affected the UrbanCA performance, and 2) CA-Markov generated simulations as accurate as UrbanCA. Compared to CA-Markov, the results of UrbanCA can be better explained by the driving factors.

3.4 Scenario prediction

We further predicted urban scenarios for 2025 using the validated ABC-CA models based on CA-Markov and UrbanCA (TIP = 0.01 and LAP = 0.8). We followed previous studies (Cao *et al*. 2016, Feng and Tong 2018b) in the Yangtze River Delta and assessed the total urban area in 2025 by assuming that the next 10-year future urban growth area would be 60% of that for the last ten years. Using this assumption, the total urban area in 2025 will be 3,035 km^2 for Shanghai. The starting map for our scenario prediction was the 2015 actual urban pattern. Each ABC-model was run for 10 iterations to create the 2025 scenarios where an iteration denotes one year.

Figure 10 shows distinct differences among the four scenarios created by CA-Markov and UrbanCA, reflecting the effect of different constraints (DIST, ROAD and POP) on future urban patterns. Meanwhile, there are fewer differences between CA-Markov and UrbanCA where the two scenarios emphasize the same driving factor. In all four scenarios, there is more urban growth in the west and south than in the eastern parts and the three islands. As inferred by the landscape metrics (Table 5), there are more 2015–2025 urban growth patches for CA-Markov than for UrbanCA, suggesting that UrbanCA tends to generate more compact urban patterns. With the BAU-scenario as the benchmark, we computed the landscape similarities among the urban scenarios. These

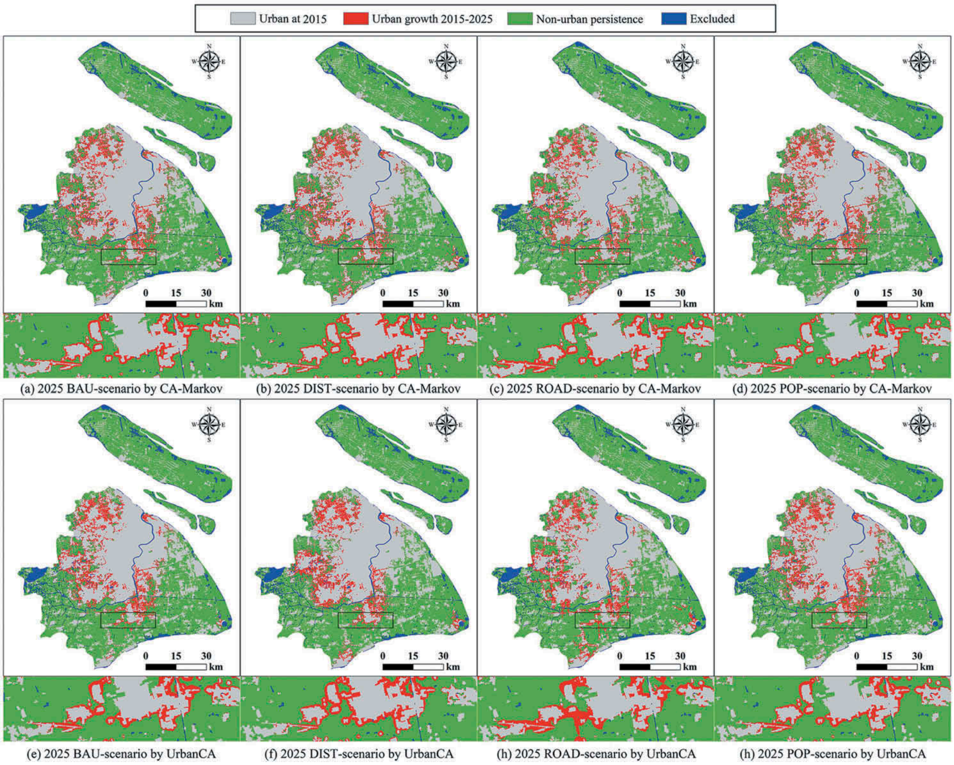

Figure 10. 2025 Shanghai urban scenarios predicted by CA-Markov and UrbanCA.

Table 5. Landscape metrics for the 2025 scenarios where the BAU-scenario serves the benchmark for computing landscape similarity.

Model	Scenario	NP	LPI	ED	LSI	AREA_MN	PAFRAC	ENN_MN	Landscape similarity
CA-Markov	BAU	5579	1.05	11.97	94.20	8.55	1.39	129.71	100.0
	DIST	5626	1.03	12.15	95.64	8.48	1.39	132.12	98.7
	ROAD	5497	0.49	11.80	92.95	8.68	1.38	125.75	91.0
	POP	5732	0.97	12.12	95.37	8.32	1.39	127.87	97.5
UrbanCA	BAU	4180	1.24	9.40	74.01	11.43	1.34	186.56	100.0
	DIST	3753	1.53	8.74	67.74	13.12	1.35	168.95	89.3
	ROAD	3670	0.50	8.74	68.18	13.29	1.33	176.34	84.3
	POP	4802	1.15	10.30	78.67	10.58	1.35	189.96	93.2

show that the ROAD-scenario is less similar to the BAU-scenario for both CA-Markov and UrbanCA. UrbanCA generated alternative scenarios that have larger differences (smaller landscape similarities) from the BAU-scenario as compared with CA-Markov. It should be noted that, however, the differences among predictions are not as significant as those implied by the land transition probability maps. This indicates that the probability map is not the only factor that affects the outcomes. The parameters and approaches implemented in the model run can significantly affect the simulation results. Therefore, the amelioration in modeling accuracy should be very limited by only improving the transition probability.

Our predictions show that both the modeling tools can successfully project urban future scenarios under different conditions where UrbanCA generated more compact urban patterns. CA-Markov can simulate and predict urban patterns, but it is limited to logistic regression and MCE methods for retrieving land transition probability maps. In this study, we applied UrbanCA to produce the ABC-based land transition probability that cannot be retrieved using CA-Makrov; that is, the land transition probability maps applied in CA-Makrov were from UrbanCA. Our UrbanCA package incorporates a number of new CA models and has stronger simulation and prediction power, providing a competitive advantage as compared to CA-Markov.

4. Discussion and conclusions

Urban modeling and scenario prediction can improve our understanding of urban growth dynamics, help optimize urban planning schemes and regulations, and propose early warnings of urban encroachment on agricultural and ecologically valuable land. Useful urban simulations need a comprehensive, robust, and efficient modeling framework with CA models that can accurately capture urban land change. While there are many CA models of urban growth, two major limitations exist as discussed in the introduction and freely available software does not provide sufficient choices of modeling approaches in practice. Moreover, some of the existing CA packages require modelers to code their programs or draw support from other software if they want to develop new CA models, compromising the convenience of using the software. New methods such as spatial statistics and heuristics in UrbanCA are definitely interesting to modelers and urban planners to produce more accurate simulations and alternative predictions.

We developed an improved CA modeling tool named UrbanCA (doi.org/10.13140/RG.2.2.11335.14242), which is available for free use. The contribution of our study is the development of new CA models and new modeling tool. This study demonstrates that: 1) the proposed mechanism for probability scaling and neighborhood scaling can effectively increase the flexibility of CA modeling, and a careful test is needed to define appropriate scaling parameters, 2) the inclusion of land use regulation layers can help examine the effects of urban planning regulations, and the incorporation of landscape heterogeneity maps can substantially reflect the urban growth anisotropy, 3) the proposed statistical and heuristic methods can provide modelers with more choices to construct different CA models, and 4) the inclusion of different validation methods can comprehensively assess the CA models. Our UrbanCA improves the methodology of CA modeling and is a worthwhile complement to existing CA simulation tools. The statistical and heuristic CA models in UrbanCA can be easily calibrated, and our tool is readily applicable elsewhere to simulation and prediction of urban future scenarios.

To examine the effectiveness of this tool, we compared it with CA-Markov using the same ABC-CA models with the modeling practice in Shanghai. For both 2005 calibration and 2015 validation, the most important metrics including overall accuracy, FOM and Ksimulation show that UrbanCA and CA-Markov have similar ability to generate past and future urban patterns when they use the same CA models; however, UrbanCA is better than CA-Markov regarding the driving factor's ability to explain the simulations. The predictions in 2025 demonstrate that UrbanCA predicted urban scenarios that are more different from each other than those generated by CA-Markov. This demonstrates the advantage of UrbanCA to decease the average landscape similarity among future alternative scenarios compared with CA-Markov. We conclude that the statistical and heuristic methods, and the proposed scaling mechanism, in UrbanCA are more useful for multi-objective modeling and multi-scenario prediction of urban development under complex conditions.

Limitations exist in the application of UrbanCA as the model implementation needs ArcGIS licensing, and the present UrbanCA tool focuses on modeling urban growth from non-urban to urban. Future work should modify this framework using free Geospatial Data Abstraction Library, and expand the modeling capabilities of UrbanCA from urban growth to multiple land use change and large-scale environmental phenomena.

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Disclosure statement

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