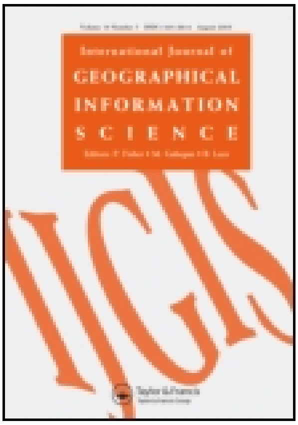

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Landscape metrics have been widely used to characterize geographical patterns which are important for many geographical and ecological analyses. Cellular automata (CA) are attractive for simulating settlement development, landscape evolution, urban dynamics, and land-use changes. Although various methods have been developed to calibrate CA, landscape metrics have not been explicitly used to ensure the simulated pattern best fitted to the actual one. This article presents a pattern-calibrated method which is based on a number of landscape metrics for implementing CA by using genetic algorithms (GAs). A *Pattern-calibrated GA–CA* is proposed by incorporating percentage of landscape (*PLAND*), patch metric (*LPI*), and landscape division (*D*) into the fitness function of GA. The sensitivity analysis can allow the users to explore various combinations of weights and examine their effects. The comparison between *Logistic-CA*, *Cell-calibrated GA–CA*, and *Pattern-calibrated GA–CA* indicates that the last method can yield the best results for calibrating CA, according to both the training and validation data. For example, *Logistic-CA* has the average simulation error of 27.7%, but *Pattern-calibrated GA–CA* (the proposed method) can reduce this error to only 7.2% by using the training data set in 2003. The validation is further carried out by using new validation data in 2008 and additional landscape metrics (e.g., Landscape shape index, edge density, and aggregation index) which have not been incorporated for calibrating CA models. The comparison shows that this pattern-calibrated CA has better performance than the other two conventional models.

Keywords: genetic algorithms; landscape metrics; cellular automata; calibration; land use

1. Introduction

In the twentieth century, rapid urbanization and urban expansion have become typical geographical phenomena around the world because of economic development and population growth. The urban population increased from 220 million in 1900 to 732 million in 1950 (29% of the world's population), and to 3.3 billion (the first time in history over half of the world's population) in 2007 (Potsiou 2010). The growth trend continues into the twenty-first century as 60% of the world's population will be urbanized by 2030 according to the report. This rush to the cities has resulted in unprecedented urban expansion and land-use changes in many fast-growing regions associated with severe ecological, economic, and social problems.

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Global environmental challenges have attracted researchers to develop advanced computer-based modeling and analysis tools to study the complex global and regional problems (Parker *et al*. 2003). Land-use change models have been developed as a useful tool to tackle these land-use problems. Simulation and prediction of urban and land-use changes can provide a new approach to support the planning and management in these fast-growing regions. This can help to facilitate sustainable development and smart growth, and improve our knowledge on the process of urbanization and its driving forces (Herold *et al*. 2003). Modeling urban development and land-use changes allows decision makers to have improved ability to assess and compare future growth and to create planning scenarios under different urban planning and management policies (Klosterman 1999, Li and Yeh 2000).

It is well recognized that bottom-up simulation models can have better performances on modeling the dynamics of many geographical systems than top-down equation-based models (Batty and Xie 1994, Clarke *et al*. 1994, Parker *et al*. 2003, Li 2011). A major drawback of equation-based models is that they have difficulties in tackling a series of complex behaviors associated with natural systems. For example, diffusion of disease, wildfire spread, ecological evolution, transport and residential development, urban dynamics, and land-use changes are usually very complex and often include nonlinear and emergent behaviors, stochastic components, and feedback loops over spatial and temporal scales (Li 2011).

As one common type of simulation methods, cellular automata (CA) have been popularly used for modeling complex geographical and ecological processes, such as rangeland dynamics (Li and Reynolds 1997), the fluctuation of animal population (Couclelis 1988), settlement changes (Deadman *et al*. 1993), evolution of cities (Batty and Xie 1994), wildfire diffusion (Clarke *et al*. 1994), land-use conversion (White *et al*. 1997, Li and Yeh 2002), forest succession or vegetation dynamics (Alonso and Sole 2000, Favier and Dubois 2004), and other ecological changes (Wang and Zhang 2001). Another type of simulation methods, agent-based models (ABMs), have also been considered more fashionable than CA because of their flexibility in addressing behaviors of individuals. However, the implementation of ABM requires sophisticated techniques, such as sample surveys, participant observation, and model configuration and calibration (Li 2011). CA are still an important and convenient tool in the simulation of urban dynamics and land-use changes for large areas (e.g., at provincial and national scales).

CA should be calibrated if they are used to simulate various geographical phenomena (Li and Yeh 2002, Silva and Clarke 2002, Straatman *et al*. 2004). Torrens and O'Sullivan (2001) argue for the development of stronger calibration techniques for CA because these models are usually calibrated by manual tuning of transition rules (Straatman *et al*. 2004). It was reported that fine tuning of CA would take much longer time in detailed applications by using a manual method (White 1995). Moreover, many calibration methods are developed according to the cell-by-cell basis. The calibration becomes rather complicated if CA are calibrated according to aggregated landscape metrics. The dilemma is that the simulation results are expected to be known prior to calculating these metrics which are required for calibrating these models.

Actually, landscape metrics have been widely used to represent urban land-use structures and land-cover changes for validating simulation models (Herold *et al*. 2002). It is considered that spatial metrics for urban and regional models can capture the structures and patterns in an urban landscape (Parker *et al*. 2001, 2003). Studies have indicated that spatial metrics are important for a variety of urban models because these metrics can help link the economic processes with the associated patterns of land use

(Herold *et al*. 2005). For example, the pattern outcomes in an ABM of edge–effect externalities can be measured by a series of landscape metrics, such as landscape composition, diversity, dominance, edge distance, edge density, shape, nearest-neighbor distance, patch number, patch size and its standard deviation, patch density, and contagion (Parker and Meretsky 2004). Recently, development patterns have also been linked to other ecological and environmental processes, such as ecological protection (Li *et al*. 2011) and energy consumption (Chen *et al*. 2011).

Most of these CA models just use landscape metrics to validate their simulation results instead of calibrating them. For example, landscape metrics are used to examine whether the simulated patterns can be fitted to the observed ones (Sui and Zeng 2001). There are very limited studies on explicitly incorporating these metrics into the calibration procedure. Attempts have been made to search for the optimized parameters of CA by using the brute-force method (Silva and Clarke 2002) and a trial-and-error procedure (Soares-Filho *et al*. 2002). The brute-force method was used to find the parameters of SLEUTH model of CA (Silva and Clarke 2002). In their experiments, the model code tried many of the combinations and permutations of the control parameters and performed multiple runs from the seed year to the present (last) data set. In each run, the calibration computed 13 different measures of the goodness of fit between the simulated pattern and the actual one. Filho *et al*. (2002) also proposed a trial-and-error method to calibrate CA according to a set of landscape structure measures, such as fractal dimension, contagion index, and the number of patches for each type of land-use and land-cover class. In the calibration, several simulation series were run by adopting the empirical transition rates and varying the mixture of the transitional functions. These methods may be very computation intensive. For example, the brute-force calibration of SLEUTH needs to yield 13 metrics of goodness of fit of the simulated pattern for the multiple runs of calibration (Onsted and Clarke 2011). In their two experiments, the calibration took 39.8 days and 70 days to complete by using the computers of an Intel Dual Core PC with two CPUs at 2.13 GHz and a Dell Precision 690 PC with a CPU at 2.33 GHz, respectively. It is attractive if CA can be calibrated by using more intelligent and efficient methods rather than the brute-force or the trial-and-error methods.

The calibration is to determine the parameters of CA based on training data. Land-use dynamics is a function of social, economic, and physical factors, which are referred to as driving forces. The contribution of each factor to land-use conversion is usually quantified by a weight in the modeling. This is the main reason that logistic regression is commonly used to derive the optimal weight of each factor. The regression will allow the predictions fitted to the known results statistically (Verburg *et al*. 2004).

Besides logistic regression, genetic algorithms (GAs) can be used to find the optimized parameters of CA (Li *et al*. 2008). GAs are an evolutionary approach consisting of two main operators: crossover and mutation. These operators are crucial for improving the fitness of a population (individuals or solutions) so that the initial guesses can be improved toward convergence at the global optimum (Tseng *et al*. 2008). GAs have been used to solve a variety of geographical optimization problems, such as site selection (Openshaw and Openshaw 1997, Li and Yeh 2005), land-use planning (Stewart *et al*. 2004), spatial geometry optimization (Brookes 2001), and multi-objective spatial search (Xiao *et al*. 2002). Recently, initial attempts have been made by using GA to calibrate CA (Li *et al*. 2008). However, this method has not used landscape metrics in the calibration so that the simulated pattern can be best fitted to the actual one. We argue that CA can be calibrated based on various landscape metrics during the multiple runs (trial solutions) from the seed year to the present (last) data set.

This article will demonstrate the necessity of developing pattern-calibrated CA if the objective is to simulate natural phenomena, such as land-use dynamics. The methodology is developed based on a common type of urban simulation models, *logistic-CA*. Although logistic regression can be used to calibrate CA, the calibration relies on cell-by-cell samples instead of aggregated landscape metrics. In this study, we will solve the pattern-based (landscape metric-based) calibration problem by using GAs. In the calibration, a special fitness function is designed to include three important landscape metrics, as well as the per-pixel accuracy during the multiple runs (trial solutions) of GA. We will compare this proposed method with the conventional methods in terms of simulation performances. Validation is carried out by using an additional classified remote-sensing image and new landscape metrics which have not been included for building the calibrated model.

2. Methodology

We will first discuss the method of logistic regression for CA calibration. However, logistic regression which is just based on per-cell samples (labeled land-use data) cannot incorporate aggregated landscape metrics into the regression. Actually, *logistic-CA* adopts a single run of calibration by using logistic regression. Therefore, we then use another method, GAs, to obtain the optimized parameters of CA (Li *et al*. 2008). In this study, we further present a pattern-calibrated CA by applying GA to *logistic-CA*. This proposed method can incorporate a number of landscape metrics during the multiple runs (trial solutions) of GA. Although the basic CA is *logistic-CA*, this method is applicable to other CA models. Replacing *logistic-CA* with other CA models is simple under the GA framework. The GA program is independent of CA because CA only provide the simulation results as the inputs to the fitness function of GA. The details of these three methods are described in the following sections.

2.1. Classical cell-calibrated logistic-CA

In *logistic-CA*, logistic regression is used to obtain the relative weights of driving forces or explanatory variables. These variables at a site are often estimated according to the accessibility to built and natural amenity features, and the neighborhood and site conditions (Conway and Wellen 2011). The accessibility in terms of proximity (attraction) factors can be regarded as the proxies of very driving forces for influencing land-use changes (Wu 2002, Li *et al*. 2008, 2011). For example, land development probability is related to the proximities to urban centers, facilities, and transportation (Wu 2002). Since land-use conversion is in a binary form (converted or not), it is straightforward to estimate the conversion probability by using a logistic form:

$$p_{ij}^t(S = \text{Converted}) = \frac{\exp\left(z_{ij}^t\right)}{1 + \exp\left(z_{ij}^t\right)} = \frac{1}{1 + \exp\left(-z_{ij}^t\right)} \tag{1}$$

where p_{ij}^t is the conversion probability at time t for cell ij; S is the state (e.g., converted or not), $z_{ij}^t = a_0 + a_1x_1 + a_2x_2 + \cdots + a_mx_m + \cdots + a_Mx_M$; a_0 is the constant; x_m is a spatial variable (e.g., distance to town centers or roads); and a_m is the parameter (weight) of this variable.

Equation (1) can be further revised to include the neighborhood function and site conditions (constraints). By considering all these factors, the *logistic-CA* is formalized by using the following equation (Li *et al*. 2008):

$$p_{ij}^{t}(S = \text{Converted}) = (1 + (-\ln\gamma)^{\alpha})\frac{1}{1 + \exp(-z_{ij}^{t})} \times f(\Omega_{ij}^{t}) \times \text{con}(s_{ij}^{t}) \tag{2}$$

where γ is a stochastic factor ranging from 0 to 1, α is a parameter to control the stochastic degree, $f(\Omega_{ij}^{t})$ is the development intensity in the neighborhood of Ω_{ij}, and $\text{con}(s_{ij}^{t})$ is the constraint score ranging from 0 to 1. The constraint score can be set according to experiences and site conditions. For example, this score should be assigned as 0 for water and steep hilly areas because land development is impossible in these strictly constrained areas.

At each iteration of simulation, p_{ij}^{t} is compared with a threshold value to determine whether a non-urbanized cell will be converted into an urbanized cell:

$$S_{ij}^{t+1} = \begin{cases} \text{Converted}, & p_{ij}^{t} \geq p_{\text{threshold}} \\ \text{NonConverted}, & p_{ij}^{t} < p_{\text{threshold}} \end{cases} \tag{3}$$

where $p_{\text{threshold}}$ is a threshold value.

The threshold (T) is determined by using observation data or an exogenous growth model which can predict land demand. For example, this value can be estimated in such a way that the total number of converted cells will be equal to the actual one, which is calculated or projected from the observed remote-sensing data (Li and Yeh 2002).

2.2. Cell-calibrated GA–CA

GAs can be used to calibrate CA according to a cell-by-cell approach (Li *et al*. 2008). GAs were originally developed based on the concepts from Darwin's theory of 'natural selection' and 'survival of the fittest' (Holland 1975, Goldberg 1989). In the computation, the process of 'natural selection' is determined by the fitness of individuals to their environment. The fitness function which is crucial for the evolutionary process is defined exogenously according to the problem domain. For example, the fitness function can be estimated according to the cell-by-cell accuracy (overall accuracy).

In this method, all the parameters of the *logistic-CA* in Equation (1) are encoded as the chromosome (CM):

$$CM = [a_0, a_1, a_2, \ldots, x_m, \ldots, x_M, p_{\text{threshold}}] \tag{4}$$

The chromosome is to represent the parameters associated with these drivers. At each generation of the evolutionary, a trial set of parameters can be regarded as an individual of GA. The performance of an individual is assessed according to its fitness to the actual pattern. A fitness function which is domain dependent is defined to indicate the performance of an individual or chromosome (e.g., a set of parameters for CA) for solving the optimal problem. In this study, the fitness function represents the difference between the actual state (e.g., actual land use) and the predicted state which is obtained from the logistic regression. The optimal set of parameters should produce the minimum value (the least error) of the fitness function. Therefore, the fitness function is calculated according to the following equation:

$$f(x) = \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 \tag{5}$$

where y_i is the actual land use at cell i and $\hat{y}_i$ is the estimated land use at cell i, which is estimated from the logistic model.

An individual (e.g., a trial set of parameters of CA) with a higher value of the fitness function will be selected as a 'parent' to produce offspring with a larger probability according to the natural selection mechanism. In this application, a larger value of the fitness function means that the solution (a trial set of parameters) can produce the smaller difference between the predicted land use and the actual one. This reproduction process is based on two main operations: crossover and mutation. The first operator which plays a crucial role in the evolution is performed by swapping a corresponding segment of a genetic representation of the parents. The second operator chooses an individual randomly and alters one randomly chosen aspect in its bit string representation. Mutation is also important because crossover cannot introduce any new information into the population. Mutation will incorporate some degree of perturbations into the evolution by avoiding the rapid degradation of population. In each step of the optimization, crossover and mutation will be applied to the last population to form a new population. As a result, this natural selection mechanism will find the optimal set of parameters for the *logistic-CA*.

Like most of the calibration methods, this GA method does not use the pattern information for the calibration. Actually, this calibration is not too much different from the logistic calibration because both try to estimate the optimized parameters just from the per-cell training data. This means that the aggregated simulated patterns are not recursively used in the calibration. As a result, the final simulated pattern will not be best fitted to the actual one in terms of landscape metrics.

2.3. *Pattern-calibrated GA–CA*

In this article, a pattern-calibrated CA is designed by explicitly incorporating landscape metrics into the calibration (Figure 1). The crucial part of this proposed method is to calculate a number of landscape metrics during the multiple runs (generations) of GA. In each generation of GA, a trial set of parameters is obtained and the development pattern is simulated by using this set of parameters. Then, the landscape metrics of the simulated pattern will be calculated and used for calculating the utility function. This utility function will affect the next generation of exploration of GA. Through this feedback process, landscape metrics can be embedded in the calibration of CA.

The methodology is similar to that of *cell-calibrated GA–CA* except for two major differences. First, cell-based calibration methods just use per-cell samples to estimate the parameters based on GAs or logistic regression. These methods do not require recursively running CA models to know the patterns during the calibration. The proposed pattern-based calibration method has to run the simulation models many times to find the best results. Second, the fitness function in the cell-calibrated CA of using GAs only considers the cell-by-cell accuracy (the overall accuracy). Since it is impossible to simulate the exact patterns like the actual ones, the use of pattern factors is important for producing more accurate calibration. In this proposed method, the fitness function has incorporated some landscape metrics as well as the overall accuracy directly from the trial simulations of CA. In each run, landscape metrics are calculated and used to calculate the fitness function (Figure 1).

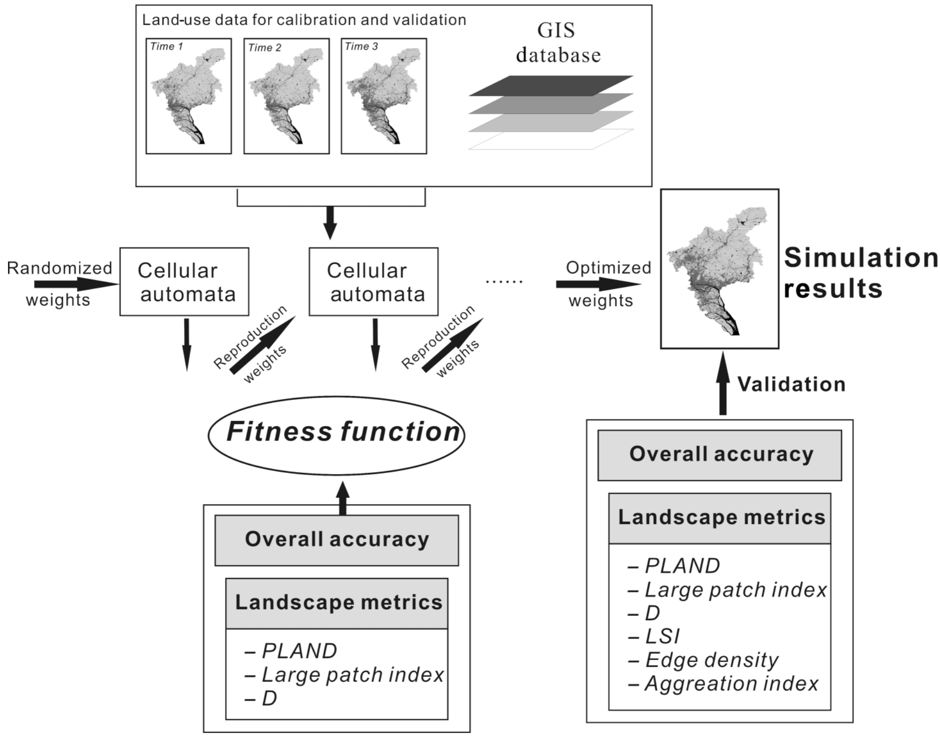

Figure 1. The methodology of the pattern-calibrated CA based on GAs.

There are many landscape metrics for characterizing geographical patterns. The first step of this proposed method is to select appropriate landscape metrics to represent land-use patterns before the calibration. During the last three decades, various landscape metrics have been proposed for geographical and ecological applications, including dominance, diversity, contagion, and fractal dimension (O'Neill *et al*. 1988, McGarigal and Marks 1995, Jaeger 2000, McGarigal *et al*. 2002). These metrics can quantify and categorize complex landscapes into identifiable patterns for understanding the process of landscape changes (Turner *et al*. 2001). However, it is unrealistic or unnecessary to use all these metrics for a single application. The selection of these metrics may be related to domain knowledge or expert preferences.

In this study, we only select three metrics for the calibration based on their importance and the experiences of previous studies. The methodology should be the same if other metrics are used instead of these three metrics. These three selected metrics are as follows: (1) percentage of landscape (*PLAND*); (2) patch metric (*LPI*); and (3) landscape division (*D*). These metrics are often used in many other studies because of their importance and usefulness (McGarigal *et al*. 2002, Batistella *et al*. 2003, Weng 2007). All these metrics are calculated at each run of GA so that a set of parameters can be obtained for a trial CA simulation. If there is a need, it is possible to include other metrics into the calibration by just changing the fitness function of GA. The modification is convenient because the fitness function is defined outside the GA program.

The first metric is percentage of landscape (*PLAND*) which quantifies the proportional abundance of each patch type in the landscape. *PLAND* is useful because it can reveal the most important information about landscape composition (Weng 2007). This indicator is calculated as follows (McGarigal *et al*. 2002):

$$PLAND = \frac{\sum_{j=1}^{n} a_{ij}}{A} \times 100 \tag{6}$$

where $i = 1, \ldots, m$ patch types (classes); $j = 1, \ldots, n$ patches; a_{ij} is the area (m^2) of patch ij, and A is the total landscape area (m^2) (adapted from McGarigal and Marks (1995)).

The second metric is largest patch index (*LPI*) which provides a measure of the size of the largest patch of a given type as a percentage of the total landscape area (Batistella *et al*. 2003). Therefore, it is a simple measure of dominance by using the following equation:

$$LPI = \frac{\max\limits_{j=1}^{a}(a_{ij})}{A} \times 100 \tag{7}$$

The third metric, landscape division (D), is a kind of fragmentation indicators. Landscape fragmentation has been considered as a major reason for the loss of species during urban development (Jaeger 2000). Landscape fragmentation creates barriers against the dispersal of species and disrupts existing ecological connections. Jaeger (2000) defined this index as the probability that two randomly chosen places in the landscape under investigation are not situated in the same undissected area:

$$D = \left[1 - \sum_{j=1}^{n} \left(\frac{a_{ij}}{A}\right)^2\right] \tag{8}$$

In the calibration, the fitness function in Equation (5) should be revised to incorporate landscape metrics as well as the overall accuracy which are calculated from each run of GA. At each run, a trial set of parameters which are obtained from GA will be used to simulate land dynamics. The assessment of the simulated pattern consists of two parts: (1) traditional cell-by-cell accuracy (overall accuracy) and (2) a combined landscape metric. Since the assessment involves multi-criteria, a well-accepted method is to combine them linearly by using the multi-criteria evaluation method (Eastman 1995, Malczewski 2006). Therefore, the proposed fitness function in Equation (5) is revised as follows:

$$f(x) = w_e \times A_{\text{overall}} + w_l \times P_{\text{land}} \tag{9}$$

where A_{overall} is the overall accuracy and P_{land} is the combined landscape metric from a trial simulation; w_e and w_l are the weights of the overall accuracy and the combined landscape metric, respectively.

The combined landscape metric is a normalized linear combination of these three indicators:

$$\begin{aligned} P_{\text{land}} = {} & |PLAND - PLAND_{\text{actual}}| / PLAND_{\text{actual}} + |LPI - LPI_{\text{actual}}| / LPI_{\text{actual}} \\ & + |D - D_{\text{actual}}| / D_{\text{actual}} \end{aligned} \tag{10}$$

where *PLAND, LPI*, and *D* are obtained from a trial simulation at each run of GA; $PLAND_{\text{actual}}$, LPI_{actual}, and D_{actual} are obtained from the classified (observed) remote-sensing images for these metrics, respectively.

All these metrics are calculated as class based at each run of GA. It is unnecessary or infeasible to implement them at patch level because each patch will grow and new patch will appear. Therefore, landscape metrics should be measured at an aggregated level (class level) for the calibration. The objective is to ensure the simulated pattern should be best fitted to the actual one at an aggregated level. At each run of GA, a trial set of parameters is obtained for CA simulation. Figure 2 shows the example that the simulated patterns of CA can be generated from different generations of GA. Then, the overall accuracy and the combined landscape metric are calculated from the simulated results. These metrics are further used to calculate the fitness function for the evolutionary approach of GA. By using this looping process, GA and CA can be fully integrated for producing the best fitted pattern. The later run (e.g., generation 100) of GA will allow CA to generate a more fitted pattern (Figure 2). This is quite different from the traditional GA–CA method in which CA is not put within GA (Li *et al*. 2008).

3. Implementation and results

3.1. Study area and spatial data

The proposed method is tested in a fast urbanized region, Guangzhou, which is situated in the Pearl River Delta, Guangdong, China. The metropolitan region of Guangzhou has an area of 7434.4 km^2. This region has been experiencing significant changes of its land-use patterns because of rapid urban expansion and population growth (Chen *et al*. 2011). Simulating urban development can provide useful information to assist urban and regional planning in this region.

Time series of satellite Landsat Thematic Mapper (TM) images of Guangzhou (Scene No. 122-44 in China Remote Sensing Ground Station reference system) were used to obtain empirical information about land-use dynamics. Supervised classification was carried out to obtain land-use classes on the TM images dated on 2000, 2003, and 2008, respectively (Chen *et al*. 2011). These images were first radiometrically and geometrically corrected before the classification. These corrected images were then classified by using a series of techniques, such as object-based classification, manual editing, and intensive field labeling with GPS. The average classification accuracies for these images are about 83–85% according to field checking (Chen *et al*. 2011).

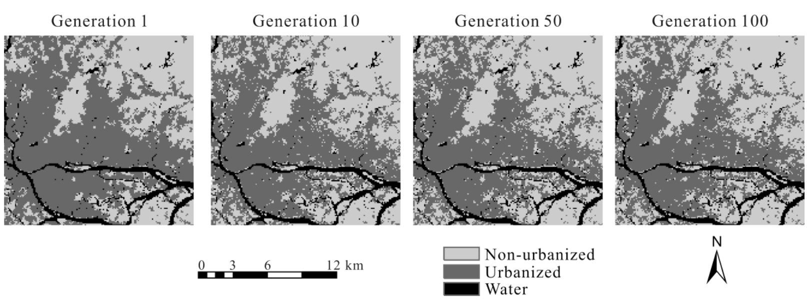

Figure 2. Simulated patterns of CA generated by a run (generation) of GA.

These classified images reveal the fast urban expansion and land-use changes in the study area. The empirical information about land-use changes obtained from classified remote-sensing images is often used to calibrate and validate CA (Li and Yeh 2002, Wu 2002). In this study, the CA model was calibrated by using the first two classified TM images in 2000 and 2003 and was further validated by using a later classified image in 2008.

A number of proximity variables which represent the attraction factors for land-use conversion should be acquired to implement the CA model (White *et al*. 1997, Wu 2002, Conway and Wellen 2011, Li *et al*. 2011). In this study, these proximity variables in Equation (1) include the distance to the main center ($x_{\mathrm{MainCenter}}$), the distance to the district centers ($x_{\mathrm{DistrictCenter}}$), the distance to the large town centers ($x_{\mathrm{LTownCenter}}$), the distance to the small town centers ($x_{\mathrm{STownCenter}}$), the distance to the railways (x_{Railways}), the distance to the subways (x_{Subways}), the distance to the expressways ($x_{\mathrm{Expressways}}$), and the distance to the roads (x_{Roads}) (Wu and Webster 1998, Li *et al*. 2008). These eight variables were generated by using common GIS functions (Figure 3).

3.2. Calibration and validation

The calibration was carried out for the three CA models described in Section 2. These models are (1) the classical *logistic-CA* based on cell-by-cell calibration (*Cell-calibrated logistic-CA*); (2) genetic algorithm CA based on cell-by-cell calibration (*Cell-calibrated*

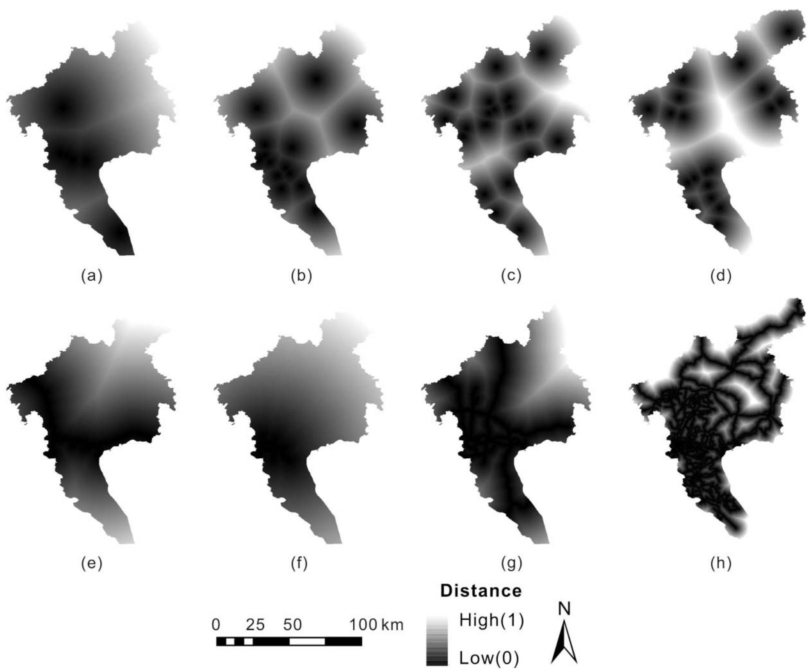

Figure 3. Various proximity variables related to Guangzhou urban dynamics: (a) distance to the main center, (b) distance to the district centers, (c) distance to the large town centers, (d) distance to the small town centers, (e) distance to the railways, (f) distance to the subways, (g) distance to the expressways, and (h) distance to the roads.

GA–CA); and (3) genetic algorithm CA based on pattern calibration (*Pattern-calibrated GA–CA*).

First, logistic regression was carried out to obtain the parameters of *Cell-calibrated logistic-CA*. The regression is to determine these parameters (weights) statistically after the dependent variable (land-use change) and the independent spatial variables (e.g., proximity variables) have been provided. The calibration was automatically implemented by using the GeoSOS free software which was developed by Li and his team (Li *et al*. 2011). This software will randomly select 20% of samples from classified remote-sensing images for the logistic regression. The combined variable (z_{ij}^t) of the *logistic-CA* described in Equation (2) was finally specified as follows:

$$z_{ij}^t = 1.222 - 2.037x_{\text{MainCenter}} + 1.035x_{\text{DistrictCenter}} + 0.293x_{\text{LTownCenter}} - 0.504x_{\text{STownCenter}} - 2.541x_{\text{Railways}} + 0.708x_{\text{Subways}} - 1.387x_{\text{Expressways}} - 3.543x_{\text{Roads}} \tag{11}$$

where $x_{\text{MainCenter}}$, $x_{\text{DistrictCenter}}$, $x_{\text{LTownCenter}}$, $x_{\text{STownCenter}}$, x_{Railways}, x_{Subways}, $x_{\text{Expressways}}$, and x_{Roads} represent the distance to the main center, the distance to the district centers, the distance to the large town centers, the distance to the small town centers, the distance to the railways, the distance to the subways, the distance to the expressways, and the distance to the roads, respectively.

Second, GAs were also used to estimate the parameters of *logistic-CA*. The weights in the combined variable (z_{ij}^t) in Equation (2) are encoded as the chromosome (*CM*):

$$CM = [a_0, a_{\text{MainCenter}}, a_{\text{DistrictCenter}}, a_{\text{LTownCenter}}, a_{\text{STownCenter}}, a_{\text{Railways}}, a_{\text{Subways}}, a_{\text{Expressways}}, a_{\text{Roads}}, T] \tag{12}$$

The chromosome is just used to represent the set of parameters for these drivers. The reason to develop GA–CA is that the landscape metrics can be later incorporated for calibrating CA. This method allows landscape metrics from the simulated patterns to be embedded within the utility function of GA. Logistic regression does not have the pattern-based calibration ability because such cell-based regression cannot use a looping procedure.

The implementation of GA needs to determine a number of parameters, such as the population size and the crossover and mutation rates. These parameters are usually decided according to users' experiences and domain knowledge. Studies indicate that the population size ranging from 20 to 200 can give a good result of the optimization for many applications (Li and Yeh 2005). In most situations, the crossover is assigned with a high probability, while the mutation with a very low probability. Like natural processes, the reproduction is mainly influenced by the crossover. The mutation only introduces a very small perturbation. In this study, the crossover rate was set to 0.90 and the mutation rate was set to 0.01. The strategy of elitist selection was also adopted that at least one of the generation's best solutions was copied without any changes to a new population. This allows the best solution to survive to the succeeding generation.

Figure 4 shows that the GA method is able to find the optimized parameters with good convergence. The fitness described in Equation (5) drops rapidly and reaches the convergence during the evolutionary approach. The search for the optimized parameters will stop when the decrease of the best fitness value is stabilized. Table 1 lists the optimized parameters of *cell-calibrated GA–CA* by using this GA method.

Finally, the GA method was also used to obtain the parameters of *Pattern-calibrated GA–CA*. The pattern calibration was based on the revised fitness function described in Equations (9) and (10). Table 2 lists the optimized parameters of this proposed model.

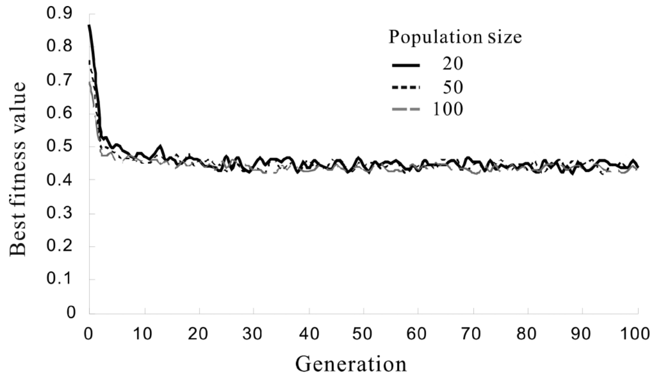

Figure 4. The relationships between the best fitness value, generation, and population size.

Table 1. The parameters of *Cell-calibrated GA–CA*.

Parameters	a_0	$a_{\text{MainCenter}}$	$a_{\text{DistrictCenter}}$	$a_{\text{LTownCenter}}$	$a_{\text{STownCenter}}$
	4.917	0.930	3.210	3.228	2.012
Parameters	a_{Railways}	$a_{\text{Expressways}}$	a_{Subways}	a_{Roads}	T
	0.397	1.913	3.185	4.828	0.433

A simple comparison can find that the parameters of traditional *Logistic CA*, *Cell-calibrated GA–CA*, and *Pattern-calibrated GA–CA* are quite different, although they share the same logistic form.

The performance of these three CA models was assessed according to the goodness of fit between the simulated pattern and the actual one which was obtained from the classified TM image in 2003. The best model should have the best goodness of fit in terms of landscape metrics as well as the overall accuracy. Tables 3 and 4 show the comparison of these three models. It is found that *Logistic-CA* and *Cell-calibrated GA–CA* have similar simulation performances in terms of accuracies measured by these indicators. However, the proposed model, *Pattern-calibrated GA–CA*, can significantly improve the simulation performances. Its simulated pattern is closer to the actual one in terms of *PLAND* and *LPI* than the other two methods. Compared with the actual pattern, for example, *Logistic-CA* (the common method) has the average error of 27.7%, but *Pattern-calibrated GA–CA* (the proposed method) can reduce this error to only 7.2%. The improvement is as high as 285.8%

Table 2. The parameters of *Pattern-calibrated GA–CA*.

Parameters	a_0	$a_{\text{MainCenter}}$	$a_{\text{DistrictCenter}}$	$a_{\text{LTownCenter}}$	$a_{\text{STownCenter}}$
	1.324	1.296	0.524	−0.936	0.841
Parameters	a_{Railways}	$a_{\text{Expressways}}$	a_{Subways}	a_{Roads}	T
	−0.520	0.976	2.897	2.329	0.867

Table 3. Calibration errors of the three models compared with the actual land use in 2003: landscape metrics and overall accuracy.

Metrics	*Actual*	*Logistic- CA*	*Cell-calibrated GA–CA*	*Pattern-calibrated GA–CA*
PLAND	11.896	13.633	15.591	11.912
LPI	3.011	5.426	5.720	3.367
D	0.999	0.997	0.996	0.999
Overall accuracy	1.000	0.841	0.867	0.833

Table 4. Calibration errors of the three models compared with the actual land use in 2003: differences compared with the actual land use.

Metrics	*Logistic-CA* (%)	*Cell-calibrated GA–CA* (%)	*Pattern-calibrated GA–CA* (%)
PLAND	14.6	31.1	0.1
LPI	80.2	90.0	11.8
D	0.2	0.3	0.0
Overall accuracy	15.9	13.3	16.8
Average error	27.7	33.6	7.2

by using the proposed method. This is because the traditional method has not taken landscape metrics into consideration during the calibration. The effects of the improvement can be easily identified by visually comparing the simulation results with the actual one (Figures 5 and 6). In the zoom-in selected areas (Figure 6), for example, *Pattern-calibrated GA–CA* can produce much better simulated patterns within the yellow circles than the other two models.

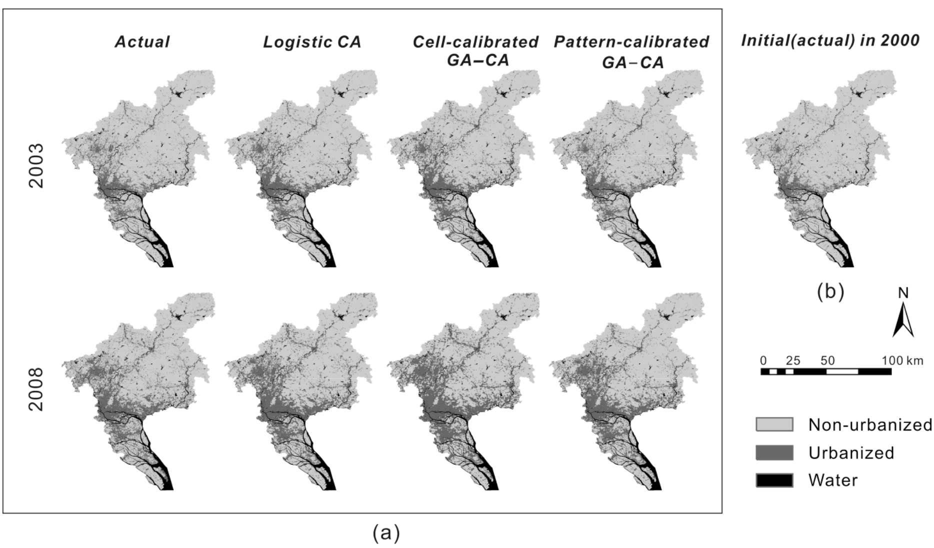

Figure 5. Simulation of urban growth for Guangzhou in 2003 and 2008.

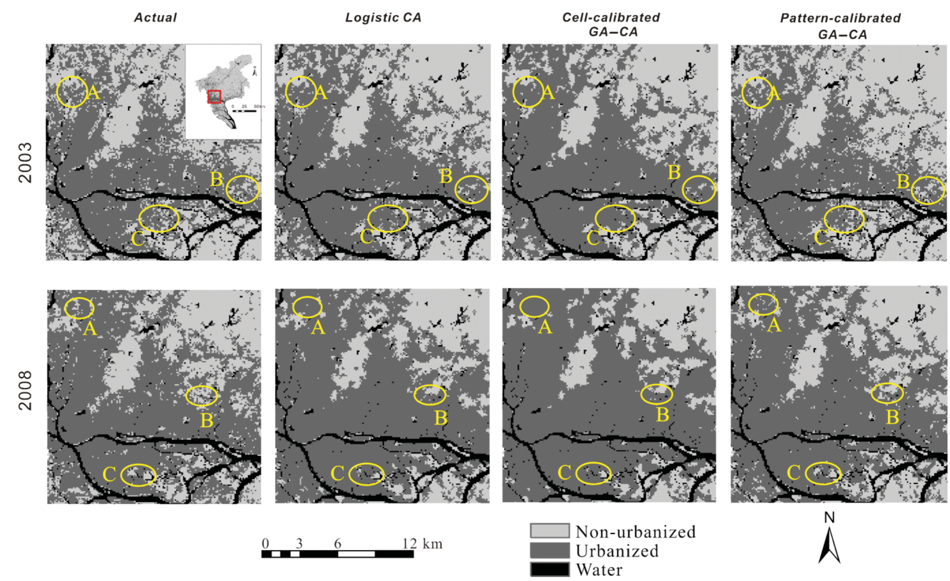

Figure 6. Comparison of simulated patterns in 2003 between *Logistic CA*, *Cell-calibrated GA–CA,* and *Pattern-calibrated GA–CA*.

The metrics in Tables 3 and 4 were obtained by using the training data in 2003. A further comparison is necessary by using the validation data in 2008 which have not been used for building these calibrated models. The comparison was carried out by assessing their accuracies in predicting urban development in 2008. The results indicate that *Logistic-CA* and *Cell-calibrated GA–CA* have similar simulation performances for these metrics. However, *Pattern-calibrated GA–CA* yields a much better results than *Logistic-CA* and *Cell-calibrated GA–CA* for the indicators of *PLAND* and *LPI* (Tables 5 and 6). Compared with the actual pattern, *Logistic-CA* (the common method) has the average error of 31.57% in terms of these four metrics, but *Pattern-calibrated GA–CA* (the proposed method) can reduce this error to only 14.0%. The improvement is as high as 124.7%. The improvement in predicting the development patterns in 2008 can be also identified by visually comparing these simulation results in the zoom-in selected areas in Figure 6.

The fitness function in Equations (9) and (10) is crucial to the identification of optimized parameters of CA. This function consists of two major components, traditional cell-by-cell accuracy (overall accuracy) and a combined landscape metric. Two weights, w_e and w_l, are used to reflect the importance of each component in the optimization. Actually, these weights can be decided according to users' preferences or planning objectives. For

Table 5. Validation errors of the three models compared with the actual land use in 2008: landscape metrics and overall accuracy.

Metrics	*Actual*	*Logistic-CA*	*Cell-calibrated GA–CA*	*Pattern-calibrated GA–CA*
PLAND	20.940	22.924	27.498	21.679
LPI	6.226	11.934	13.487	7.914
D	0.995	0.985	0.981	0.992
Overall accuracy	1.000	0.760	0.787	0.748

Table 6. Validation errors of the three models compared with the actual land use in 2008: differences compared with the actual land use.

Metrics	*Logistic-CA* (%)	*Cell-calibrated GA–CA* (%)	*Pattern-calibrated GA–CA* (%)
PLAND	9.5	31.3	3.5
LPI	91.7	116.6	27.1
D	1.0	1.4	0.3
Overall accuracy	24.0	21.3	25.2
Average error	31.5	42.7	14.0

example, the weight of w_l should be assigned with a larger value if the pattern factor is more important than the overall accuracy in the calibration.

If these weights are unclear to users, sensitivity analysis can be carried out to assist the determination of these weights. In the above experiments, the same weight (e.g., $w_e = 0.5$ and $w_l = 0.5$) is given to these two components. However, these weights can be varied to examine their effects on simulation. It is clear that the optimized parameters of CA are affected by using different combinations of w_e and w_l in the fitness function. The combination, $w_e = 1$ and $w_l = 0$, is equivalent to the setting of the traditional method which ignores the component of landscape metrics. Such a combination may produce a quite different pattern from the actual one in terms of landscape metrics. Table 7 shows the results of the sensitivity analysis by using different combinations of w_e and w_l. It is ideal that a simulated pattern should have the best fit to the actual one. The proposed method may help to achieve such a goal by considering all the options in an evolutionary approach.

In the above GA method, the pattern calibration only considers three important landscape metrics, percentage of landscape (*PLAND*), patch metric (*LPI*), and landscape division (*D*). There is a question if such pattern-calibrated model can produce good performances if other landscape metrics are used for the validation. Therefore, we further introduce three new metrics which are not included in the calibration for a more robust validation.

The first new metric is landscape shape index (*LSI*) which is a simple measure of class aggregation or clumpiness of a pattern. This metric is given by the following equation (McGarigal and Marks 1995):

$$LSI = \frac{e_i}{\min e_i}$$

Table 7. Sensitivity analysis by using different combinations of w_e and w_l.

		Scenario				
Metrics	*Actual*	$w_e = 1$, $w_l = 0$	$w_e = 0.75$, $w_l = 0.25$	$w_e = 0.5$, $w_l = 0.5$	$w_e = 0.25$, $w_l = 0.75$	$w_e = 0$, $w_l = 1$
PLAND	11.896	15.591	12.995	11.912	11.918	11.908
LPI	3.011	5.720	4.368	3.367	3.248	3.238
D	0.999	0.996	0.998	0.999	0.999	0.999
Overall accuracy	1.000	0.867	0.846	0.833	0.824	0.823

where e_i is the total length of edge (or perimeter) of class i in terms of number of cell surfaces (including all landscape boundary and background edge segments involving class i) and min e_i is the minimum total length of edge (or perimeter) of class i in terms of number of cell surfaces.

The second new metric is edge density (*ED*) which reports the edge length on a per unit area basis. This metric can facilitate comparison among landscapes of varying size. This metric is defined as follows (McGarigal and Marks 1995):

$$ED = \frac{\sum_{k=1}^{m} e_{ik}}{A} \times 10,000$$

where e_{ik} is the total length (m) of edge in landscape involving patch type (class) i (including landscape boundary and background segments involving patch type i) and A is the total landscape area (m^2).

The last metric is aggregation index (*AI*) which is calculated from an adjacency matrix. This metric shows the frequency with which different pairs of patch types appear side by side on the map. The following equation is used to represent this metric (He *et al*. 2000):

$$AI = \left[\frac{g_{ii}}{\max g_{ii}}\right] \times 100$$

where g_{ii} is the number of like adjacencies (joins) between pixels of patch type (class) i based on the single-count method, and max g_{ii} is the maximum number of like adjacencies (joins) between pixels of patch type (class) i based on the single-count method.

The validation based on these three new metrics was carried out for the simulated patterns in 2003 and 2008. The results are very plausible according to the comparison in Tables 8 and 9. It is found that *Pattern-calibrated GA–CA* can produce the values of *LSI*, *ED*, and *AI* much closer to those of the actual patterns in 2003 and 2008 than the other two

Table 8. Validation of the three models based on new metrics: validation based on new landscape metrics for 2003.

Metrics	*Actual*	*Logistic-CA*	*Cell-calibrated GA–CA*	*Pattern-calibrated GA–CA*
LSI	76.003	63.249	59.240	69.340
ED	5.000	4.526	4.532	4.644
AI	60.937	70.245	73.990	64.999
Average error (%)	100	13.8	17.6	7.5

Table 9. Validation of the three models based on new metrics: validation based on new landscape metrics for 2008.

Metrics	*Actual*	*Logistic-CA*	*Cell-calibrated GA–CA*	*Pattern-calibrated GA–CA*
LSI	80.171	60.194	51.196	66.375
ED	7.168	5.450	5.204	5.587
AI	69.709	80.202	83.128	77.512
Average error (%)	100	15.1	19.3	11.2

models. Compared with the actual pattern, for example, *Logistic-CA*, *Cell-calibrated GA–CA*, and *Pattern-calibrated GA–CA* have the average error (in terms of these three metrics) of 13.8%, 17.6%, and 7.5%, respectively, for 2003. These values become 15.1%, 19.3%, and 11.2%, respectively, for 2008. It is obvious that the proposed method can still perform significantly better than the other two traditional methods if the validation is based on new metrics.

The proposed method needs much more time to complete than the other two methods because the landscape metrics of trial simulations are calculated at each run of GA. In our experiments, the calibration took about 40 hours to complete by using the computers of an Intel Xeon PC with two CPUs at 2.40 GHz. However, the time is much faster than that of the brute-force method. In the two experiments by Onsted and Clarke (2011), for example, the brute-force calibration took 39.8 days and 70 days to complete by using the computers of an Intel Dual Core PC with two CPUs at 2.13 GHz and a Dell Precision 690 PC with a CPU at 2.33 GHz, respectively.

4. Conclusions

CA are quite popular and convenient for simulating urban development and land-use changes in large areas. This article has demonstrated that the incorporation of landscape metrics is important for a stronger calibration of CA. It is quite difficult to produce the best fit between the simulated pattern and the actual one by using existing calibration methods. A major problem with most of these methods is that landscape metrics are not included in the calibration. Early work on the automatic calibration of CA may include the methods of logistic regression (Wu 2002) and neural networks (Li and Yeh 2002). Logistic regression should be a useful and convenient tool for calibrating CA (Wu 2002, Li *et al*. 2008, Lin *et al*. 2011). In developing a *logistic-CA*, logistic regression is used to quantify the relationships between land-use conversion and their drivers (spatial variables). In the logistic regression, the parameters associated with each spatial variable are statistically determined by using samples (cell-based data) (Pontius *et al*. 2008). However, this method has difficulties in embedding aggregated landscape patterns explicitly into the regression procedure.

Pattern-based calibration should have a great appeal for a variety of simulation models which are used to solve ecological and urban planning problems. Actually, landscape metrics can be used to quantify the spatial heterogeneity of individual patches for reflecting important spatial properties. These metrics provide important information that can characterize urban and land-use systems. These metrics are initially developed for the measurement of forest patches (Sudhira *et al*. 2004). They have become a useful quantitative measure to describe structures and patterns of a landscape. These indicators have been applied to the detection of landscape patterns, biodiversity, and habitat fragmentation; the description of changes in landscapes; and the investigation of scale effects in describing landscape structures (O'Neill *et al*. 1996, Herold *et al*. 2002).

Although the brute-force method and the trial-and-error method can be based on the pattern factors, these methods are quite computation intensive. This study presents a new method to incorporate a number of landscape metrics explicitly into GAs for calibrating CA. Unlike traditional methods, this GA–CA method allows the calibration to be based on the metrics calculated from CA simulation at each run of GA. Landscape metrics and overall accuracy are calculated each time from a trial simulation under this GA framework. In this study, three important landscape indicators, percentage of landscape (*PLAND*), patch metric (*LPI*), and landscape division (*D*), are selected for calculating the fitness function of GA. The optimization requires the looping procedure repeated many times to find the optimized parameters of CA so that the simulated pattern can be best fitted to the actual one.

The comparison indicates that the proposed method can yield quite plausible results of simulation by using these metrics. For example, the proposed method (*Pattern-calibrated GA–CA*) yields the average simulation error of 7.2%, while the other two traditional methods have the average simulation errors of 27.7% and 33.6%, respectively, for 2003. The improvement is also significant by using the validation data in 2008, which have not been used for building the calibrated models.

The calibration involves a number of factors (e.g., landscape metrics and overall accuracy) in the fitness function. The importance of each factor is determined by its weight. The determination of these weights can be facilitated by the sensitivity analysis. This analysis allows the users to examine the effects of using different combinations of weights for these factors. Experiments were carried out by varying these weights instead of using the same weight for each factor. Although the linear combination may have drawbacks, it is quite practical and convenient for exploring different options in the search for the optimized parameters of CA.

A more robust validation is to examine whether the proposed method can perform well if the assessment is based on other new landscape metrics which are not included in the calibration. In this study, these new metrics include landscape shape index (*LSI*), edge density (*ED*), and aggregation index (*AI*). The comparison shows that *Pattern-calibrated GA–CA* still yields the best performance in terms of *LSI*, *ED*, and *AI* for simulating both the 2003 and 2008 patterns. This means that *Pattern-calibrated GA–CA* is effective in producing the pattern which is closest to the actual one.

Although the proposed method can yield quite plausible simulation results, it is subject to some assumptions and limitations. The underlying assumption behind the landscape-based approach is that any changes will not abruptly change landscape behavior. This means that the growth is based on historical trends. Although landscape metrics are incorporated into the calibration, these metrics are used at an aggregated landscape level instead of detailed patch level. Moreover, the utility function of GA is based on a linear combination of all these landscape metrics.

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