Calibrating and validating cellular automata models of urbanization

Dr. Paul M. Torrens, Associate Professor, Geosimulation Research Laboratory, School of Geographical Sciences & Urban Planning, Arizona State University, Tempe, AZ, 85287-5302, USA.

Citation: Torrens, P.M. (2011) "Calibrating and validating cellular automata models of urbanization". In Urban Remote Sensing: Monitoring, Synthesis and Modeling in the Urban Environment, Yang, Xiaojun (Ed.). Chichester: John Wiley & Sons, pp. 335-345

ABSTRACT

Automata-based modeling of urban dynamics is an active research enterprise that has gathered momentum at an increasing pace. Despite its popularity, research and development in this domain remains in a state of relative stasis, largely constrained by persistent problems in registering simulation scenarios to the real world that model developers seek to simulate. To a degree, these problems are indicative of modeling as a scientific endeavor more broadly, but application of automata models to human-environment contexts raises some particularly challenging issues for calibration and validation that the field could benefit from addressing. This chapter reviews the state-of-the-art in applying cellular automata models to human-environment interactions in complex, messy, dynamic urban systems, with all of its associated problems and promise.

KEYWORDS

Cellular automata, geosimulation, urbanization, simulation, calibration, validation, complexity

INTRODUCTION

All models are abstractions of a complicated reality and in simulation there is an imperative to assess the match between modeled phenomena and the real world. *Empirically* determining this correspondence is always somewhat of a losing proposition because of limits to what might be observed, the partiality inherent in most data-sets, discrepancy between modeled spatial and temporal scales and those of natural and social phenomena, and the non-uniqueness of any hypothesis or assumption (Oreskes et al., 1994, Batty and Torrens, 2005). These problems are exacerbated when models are used to speculate about futures, about which we can know almost nothing with certainty and they become especially problematic when we fashion models of complex systems (Allen and Torrens, 2005). Regardless of how problematic issues of mismatch might be, models are nevertheless used as research, experimental, and diagnostic tools and so treatment of their “fit” to the real world or to a purpose is significant, particularly when models are tasked to test theories or to support plans, decisions, or policies. Calibration and validation exercises are particularly significant in urban applications of models to human-environment interactions, where there has been a tradition of using computer models as planning support systems (Brail and Klosterman, 2001), often for use in determining the potential impact of infrastructure developments, human activities, and land-uses upon the environment, or even for assessing compliance with legislative rulings relating to transportation efficiency and air emissions standards (Southworth, 1995).

The terminology surrounding model-matching exercises is infamously vague and confused (Oreskes et al., 1994), but is perhaps best summarized as follows. “Verification” exercises serve to register a model (generally) to a particular application, system, place, or time, or to fit a particular purpose (normative modeling, conceptual modeling, decision support). “Calibration” involves (specifically) adjusting model parameters so that simulations (where simulation is the act of “running” a model on data or applying it to a given scenario) can be performed with a level of fitness or sufficiency for their intended purpose. “Validation” involves assessing the success of a model or simulation run in achieving its (specific) intended goals. In all cases, these exercises usually involve comparing the performance of the model to some properties of the real system being simulated. In a relative minority of cases, similar schemes are used to compare models to other models, or individual runs of a single model in varying places and times (Pontius Jr. et al., 2008, Wegener, 1994). Comparisons are commonly made against known or observed conditions.

Urban automata models, usually formed as cellular automata, individual-based models, agent-based models, or multi-agent systems (Benenson and Torrens, 2004) have become increasingly popular in human-environment research, in large part owing to their flexibility in representing an almost limitless variety of phenomena and systems. Among their advertised advantages, automata model-builders often tout the ability of automata to simulate complex dynamic systems that defy easy analysis by more traditional forms of modeling (Parker et al., 2003, Batty, 2005, Grimm, 1999, Manson, 2001). Verifying the utility of such models for the systems and uses to which they are applied in urban and environmental studies has, however, proven to be a thorny issue (Batty and Torrens, 2005, Manson, 2007, Torrens and O'Sullivan, 2001, Pontius Jr. et al., 2008).

Nevertheless, work in this area is active and it is advancing. Much of the current research emphasizes statistical procedures, which are employed in gauging uncertainty or sensitivity in empirical analysis, providing formal methodology for analyzing relationships and the strength of association between simulation output and data about the system being simulated (Pontius Jr. et al., 2008, Dragićević and Kocabas, 2007, Kocabas and Dragićević, 2006). Remotely-sensed imagery has also emerged as an important source of “dataware” for model validation and calibration, feeding models with data and providing the catalyst that allows model data output to be contextualized into information (Bone et al., 2007, Herold and Clarke, 2002, Torrens, 2006a). Increasingly, model developers are relying on spatial analysis and image processing techniques that are more usually applied to the analysis of real cities to analyze patterns and regularities in simulated cities: to extract features, examine geographic trends, analyze spatial structures, etc (Herold et al., 2005). Some of the advances in the computer sciences that enabled the introduction of automata techniques to the geographical sciences have also been employed in the calibration and validation of automata models using techniques from Artificial Intelligence (AI) (Almeida et al., 2008).

In his chapter, I review the state-of-the-art in calibration and validation of urban cellular automata models, with particular emphasis on models tasked with simulating human-environment interactions through land-use and land cover change, largely because it is in these application domains that development of automata models is advancing most rapidly. The chapter continues in the next sections with discussion of calibration mechanisms—conditional transition, weighted transition, and state-based constraints. Discussion of the derivation of values for calibration parameters follows, with particular attention to visual calibration, statistical tests, the use of historical data, regression of parameter values, the use of exogenous models, and automatic calibration procedures. The focus of this chapter then moves to consideration of model validation routines through use of visual inspection, pixel-matching, feature and pattern recognition, and the analysis of complexity signatures. Various procedures for sweeping the parameter space of models are then discussed before the chapter draws to a close with some concluding discussion.

CALIBRATION

Cellular automata models are generally calibrated by tailoring the parameters that control transition rules. In addition, calibration may be performed on a state-basis or cell-basis, allowing special conditions by which the normal state transition procedure for those states or cells might be specially treated. For system properties that might sit beyond the range of an automata simulation, external models may be used to calibrate automata parameters.

Conditional Transition Rules

Conditional transition invokes calibration by determining circumstances under which transition may or may not take place. One classic example is a so-called stopping rule, which freezes state transition to prevent a simulation from evolving beyond a particular time-step, over a geographical boundary, or outside specified state parameters. Stopping rules do have some theoretical basis. For example, in urban applications they are synonymous with holding capacity for built infrastructure or the environment; they may be associated with the notion that cities can accommodate people, vehicles, only up until a certain point or up to a particular threshold of sustainability. The actual stopping procedure can be introduced, *a priori*, or it can be context-specific, subject to evolving conditions in a simulation. In their model of urbanization in Dongguan, China, for example, Yeh and Li (2002) use population totals as a stopping rule for simulation runs. A simulation is halted when the total target ("known") population for a simulation run is reached. Alternatively, Ward and colleagues (2000a) use geographical extent as the basis for a stopping rule in their models of urbanization; once a simulation reaches a target area, urbanization ceases to proceed further.

Thresholds are another example of conditional calibration, used to establish the lower- and upper-limits for certain properties or events in a simulation run. Often, attainment of a threshold value stimulates a particular action in a simulation (a particular state transition, introduction of a new rule, initiation of a feedback loop). Transition thresholds have strong analogies with properties of real urban systems (trip-making is often governed by capacity thresholds, for example). White and colleagues (1997) use thresholds to specify a quota of total cell transitions in their simulations of urbanization. Their models are run as normal, transitioning between states on a cell-by-cell basis, until the threshold quota is reached. At that point, transition is constrained by setting the transition potential of all cells in the model to zero.

The use of transition hierarchies is another way to calibrate a model. Often, the sequence of urbanization adheres to a particular formal sequence. Vacant lots, for example, have the potential to be used for any activity; a site that was previously occupied by a heavy chemical industry, on the other hand, has limited potential for re-development because of the considerable effort required to “reclaim” it. Hierarchies are generally implemented as rankings on state transition potentials in urban models. This process operates as follows. Particular uses are ranked: states that are observed in great abundance in the system (residential land-use, for example) may be ranked on one (lower) extremity of a scale. States that feature less frequently (some form of locally unwanted land-use such as waste disposal, for example) will be ranked on another (higher) extremity of that scale. State transition can then be specified in such a way that states may only transition to other states with *higher rankings*. White and Engelen (1993) use this approach to condition land-use transition in their models. In their examples, a vacant cell may transition to *any* other use (housing, industry, commerce). A cell with a housing land-use can transition either to industrial or commercial uses. An industrial cell may transition *only* to a commercial state. The use of hierarchies thereby establishes a mechanism for plausible urban momentum.

Weighted Transition Rules

Weights are used to calibrate automata models by “elasticizing” transition rules; this allows models to amplify or dampen processes by determining the *likelihood* of an event occurring in a simulation run, or the *intensity* of its influence. Weights are commonly specified as transition potentials, controlling the likelihood of transition to a particular state. Often, the influence of several such potentials can be combined, as a *weighted sum*. Transition weights have analogies in real urban systems. Agglomeration effects are the most obvious example: colocation of particular land uses (car dealerships, for example) may establish mutual further potential for additional collocation of the same activity, say, through economies of scale, for example. The phenomenon also works inversely; certain activities act with a repellant influence: power plants, hazardous industries, disposal facilities are rarely collocated with residential land-uses (they have a negative elasticity).

Weights are particularly useful for calibrating rates of change and transition potentials for automata (Xie, 1996, Batty and Xie, 1997). Static weights remain constant over the course of a simulation run. Dynamic weights, on the other hand, may change in influence as a simulation run evolves. The most common exemplar in automata modeling is the use of growth rates. By weighting growth (or decline), the speed of evolution in a model run can be hastened, placed in relative stasis, or slowed. In a sense, growth rates set the overall metabolism for a simulation. In their model of urbanization in Cincinnati, OH, White and colleagues (1997) introduced a static, universal growth rate, which held constant over a simulation. In the SLEUTH models developed by Clarke and colleagues (Clarke, 1997, Clarke and Gaydos, 1998, Clarke et al., 1997, Clarke et al., 2007), the rate of urbanization in their simulations is linked, dynamically, to the (evolving) size (area extent) of the simulated city. As the city grows, its rate of development accelerates. As growth slows toward a standstill, the growth rate is dampened. Weighting by distance is a related approach. White and colleagues (1997) make use of a distance-dependent weight on state transition in their cellular automata models. Transition is weighted more heavily—specifically, it has a higher probability of successful transition—for cells that are closer to a specific cell. Essentially, this establishes a mechanism to temper transition by distance-decay. Elsewhere, White and colleagues (1997) introduce weights designed to mimic the attraction-repulsion effects of various land-uses on one another, designing weights to mimic agglomeration and nuisance effects and the distance-decay of those influences. Weights can also be used to introduce stochastic perturbation to model dynamics, as a proxy for unexplained (or uncertain) factors in a model. For example, White and Engelen (1993) used a weighting parameter to control the overall level of perturbation in their models. They found that their simulation runs were highly sensitive to the perturbation parameter, concluding that it was an important factor in calibrating a model to *real* applications. Yeh and Li (2002) used a random variable for stochastic perturbation, scaling (weighting, really) it to restrict it within a "normal range of fluctuation" (plus or minus ten percent).

Seeding and Initial Conditions

Urbanization often exhibits trends of path dependence around a particular condition or event. Once this pattern is "locked-in" (Arthur, 1990), it becomes relatively difficult to change the trajectory of the system to a new phase. The canonical example in urban studies is the initial settlement site for a given city, which loses significance as the city develops but retains a central position in its metropolitan hierarchy because of inertia (Hall, 1988). Similar mechanisms are used to calibrate models to known (historical) conditions. Clarke and colleagues (1997), for example, used historical maps and other data sources to identify and place the initial position of settlements in the San Francisco Bay Area. This information was then used to set seed cells for a cellular automata simulation of the area's urbanization; in a sense, it ensured that right stuff grew in the right places. They also introduced a layer of road states, employed such that once a simulation run transitioned through specific temporal markers, the appropriate road data features were read into the model. Torrens (2006b) similarly used the initial settlement pattern of the system of cities around Lake Michigan and known population totals to establish initial conditions in his model of sprawl formation in the Midwestern megalopolis. Seed constraints can also be applied in the opposite direction: the SLEUTH model, for example, has been run from contemporary seed conditions, and reversed back in time over a historical period for the Santa Barbara Region, beginning with conditions in 1998 and running back to 1929 (Goldstein et al., 2004).

Exclusion mechanisms can also be used to constrain simulations by withholding certain cells from transition consideration over a model run, or over a particular time period in a simulation. White, Engelen, and colleagues, for example, use this procedure to distinguish between “fixed” and “functional” cells in their cellular automata models. “Fixed” cells correspond to areas of a city that remain exempt from urbanization: permanent land-uses such as rivers, parks, and railways. “Functional” cells are consistent with sites that are open to urbanization; they are subject to the full range of transition rules specified in the model (White and Engelen, 2000). Clarke and colleagues similarly employ a layer of “excluded areas” in their models (Clarke et al., 2007). This layer is used to represent cells that are immune to growth processes in a simulation: ocean, lake, and “protected areas”. They also introduce topography constraints that prohibit urbanization above a given slope threshold. A similar scheme is employed in the Dynamic Urban Evolution Model (DUEM) developed by Xie and Batty (Batty et al., 1999). Li and Yeh (2002) vary this standard approach slightly in their applications: they associate development with the potential environmental costs of urban growth, excluding areas of cropland, forest, and wetland from their model. In a similar exercise, they developed mechanisms to freeze urban growth in environmentally sensitive and important agricultural areas of their simulated area, relating the constraint to ideas of sustainability (Li and Yeh, 2000).

Specifying the Value of Calibration Parameters

There are a variety of methods by which the empirical value of calibration parameters such as weights and constraints might be derived. These methodologies include visual calibration, statistical tests, the use of historical data, and statistically regressing parameter values. In addition, exogenous models may be used to supply parameter values. In recent years, several automated calibration procedures have also been developed for urban automata models.

Visual calibration involves the manual tweaking of rules by comparing simulation runs visually (Aerts et al., 2003). Essentially, a model designer or user acts as an expert system, adjusting weights and parameter values based on her observation of model dynamics: “The eye of the human model developer is an amazingly powerful map comparison tool, which detects easily the similarities and dissimilarities that matter, irrespective of the scale at which they show up. And the model developer, with all his knowledge of spatial form and spatial interaction processes, is a very able (if often unwilling) “calibration machine”” (Straatman et al., 2004). On other occasions, the values of calibration parameters have been derived from historical data sources. Most often, land-use maps are used. White and colleagues calibrated weights in their model of Cincinnati against land-use maps dating back to 1970 (White et al., 1997), for example.

Statistics may also be used to calculate parameter values. Clarke and Gaydos ran descriptive statistical tests to determine the parameter vales in their models of San Francisco, Washington D.C., and Baltimore (Clarke and Gaydos, 1998). Wu and Webster (1998) used a series of logistic regressions to calibrate the probabilities for transition rules in their model of land development in Guangzhou, China: the beta-values from a regression equation were used, directly, as the value for model weights. Similarly, in his model of polycentric urbanization, Wu (1998) introduced a transition rule (which he termed as an “action function”) that calibrated the model’s decision- and preference-based transition rules. This function was specified using a regression equation that was itself calculated based on real choice observation data. Arai and Akiyama (2004) also used regression to derive transition weights in their model of urbanization in the Tokyo Metropolitan area.

Coupling Automata and Exogenous Models

Strictly speaking, automata models should be closed systems: they should not be open to external influence. However, in some instances (and often born of a necessity to better ally with the reality that they try to emulate), urban automata models have been coupled with exogenous simulations: model output, routines, or equations external to an automata model are used to influence transition in an automata simulation, either by initiating state transition directly, or by determining the value of constraints and weights. There are a few rationales for using exogenous models in this way. Simple convenience is one reason: exogenous models can be employed to introduce mechanisms that may not be treated (or that a model-builder may not wish to treat because of disjointed time scales, for example). There are also theoretical justifications. Exogenous models can be used to represent phenomena that are external to the system of interest: non-urban sub-systems such as climate, hydrology, geology, or external (but locally relevant) phenomena such as the operation of cities in a regional system, national boom-and-bust cycles, and geo-political dynamics. The MURBANDY model developed by White, Engelen, and colleagues (Engelen et al., 2002) uses three exogenous models to establish the level of demand for cell state transition in its automata-based microsimulation of urbanization. Sea-level rises, as simulated in a natural environment model, may trigger a conversion in state variables from active land-use to inactive sea uses at low elevations, for example. Many top-down systems, such as the evolution of public policy, are very difficult to "get right" in simulation and are perhaps best handled as a given, but external, influence on system dynamics. Indeed, a model might actually have been built to evaluate the nitty-gritty system dynamics that follow on from the use of various policy "levers" on a system's trajectory.

Growth rates may also be specified exogenously, for example, when growth is assumed to originate outside a given urban system, e.g., through in-migration or as a function of economic and demographic links with other systems (Torrens, 2006b). White and Engelen (1993), for example, treated growth as external to their cellular automata models because they regarded growth in a real city as being dependent on the position of a city in its regional or national economy, rather than its internal spatial structure. However, problems may arise if exogenously-specified constraints conceal the actual interactions between local states in a CA (Straatman et al., 2004).

Automatic Calibration

Urban automata models may be specified with a bewildering array of inter-dependent parameters and widgets. Calibrating those mechanisms often requires the use of high-performance computing (Nagel and Rickert, 2001, Hecker et al., 1999, Bandini et al., 2001, Guan et al., 2006). Several authors have developed schemes for automatic calibration, typically adding calibration modularly as a step in a simulation run. A range of techniques have been employed to achieve this, including brute-force approaches, optimized search routines, and self-modification schemes.

Brute-force calibration (Silva and Clarke, 2002) is a procedure for essentially throwing computer power at a model to run it over many permutations and combinations of parameter values. Several developments to the SLEUTH model have been undertaken around these goals (Guan et al., 2006). In such instances, results of varying parameters are sorted according to some metric, and the highest-scoring results are fed into the next iteration of the procedure.

Optimized search procedures are similar to the brute-force approach, but introduce an element of machine intelligence. Unlike the brute-force approach, which rank-selects parameter values rather simply, optimized search schemes use a variety of guidelines (decision rules) to target parameter adjustments. This approach begets related issues: how to gauge error; how to formulate a decision rule (adjust up, adjust down, aim for the optimal solution, go for a less-than-optimal solution); how to choose between adjustments that appear to yield the same improvement; and what to do if the adjustment decision yields an unsatisfactory result that manifests only after several subsequent transitions have taken place. In the example developed by Straatman and colleagues (2004), a procedure was introduced that targeted searches based on benchmarks for maximum error (the neighborhood with the greatest difference between desired potential and undesired potential) and total error (the number of neighborhoods, or cell count, that resulted in a wrong state). Adjustment was carried out by means of “length searches” (adjustments that yield a result that is more likely to convene on a desired state, or less likely to result in an undesired state) and “width searches” (adjustment guided by the relative ability of the adjustment options to reduce total error). To avoid having to make random choices between similarly-optimal adjustments, a variety of techniques were proposed, including making the length and width searches inter-dependent, varying those approaches, and making use of “backtracking” (setting the adjustment procedure back by a number of transition steps, and relaxing the adjustment to allow for less-than-optimal solutions).

An alternative method for automatic calibration involves the use of self-modifying mechanisms: transition rules are allowed to change (in relative importance or weighting) as a simulation evolves. Under self-modifying calibration schemes, changes in parameter values are often linked to evolving conditions within the model itself. In the SLEUTH model, for example, the rate of growth serves as a trigger for adaptation in the application of rules (Clarke et al., 1997, Clarke, 1997, Clarke and Gaydos, 1998, Silva and Clarke, 2002, Goldstein et al., 2004, Candau et al., 2000). Under conditions of rapid growth, growth control parameters in the model are exaggerated. Essentially, this acts as a brake on the growth metabolism or momentum of the model. If a simulation exhibits “little or no growth”, the growth parameters are adjusted to dampen growth. Without self-modification of this nature, simulation runs would produce only linear or exponential growth (Silva and Clarke, 2002).

VALIDATING AUTOMATA MODELS

For the most part, model calibration takes place before a simulation run. Validation relates to the assessment of a model's performance, and this generally takes place after a simulation has been run. In abstract terms, we may differentiate between qualitative validation and quantitative validation. The former refers to the evaluation of general agreement between a simulation and observed conditions; the latter denotes the assessment of empirical goodness-of-fit between simulation outputs and observed conditions. We can also distinguish between validation mechanisms designed to assess model performance through analysis of the patterns and outputs that a simulation generates and mechanisms that analyze a simulation run itself, as a simulation of the system being considered.

Pixel Matching

Validation by visual inspection is one of the most straightforward (but subjective) techniques for assessing the performance of a model. In a sense, model designers or users act as their own expert systems in studying the system as it unfolds in simulation. For example, one might evaluate whether a model generated plausible urban forms (Wu, 1998), or whether the simulated processes operated at sensible rates and with appropriate consequences (Torrens, 2006b). In their models of urban growth in the San Francisco Bay Area, Clarke and colleagues used visual validation to determine estimates for parameter settings in the model. Simulations were run, their performance was evaluated visually, and parameters were adjusted based on those evaluations if necessary (Clarke et al., 1997). They looked, in particular, at whether their model generated realistic patterns of historical growth, and realistic urban extents. They also looked at the plausibility of area, edge, and cluster attributes in the simulation output.

One might opt, alternatively, to have a *computer* inspect the visual match between a model's output and a real-world pattern. This is usually done by pixel matching or by pattern recognition. Pattern recognition implies a targeted search—analysis to determine the presence of specific features, artifacts, or configurations that are known or spelled-out *a priori*. Pixel-matching, by contrast, is a more mechanical approach, involving the analysis of the composition of a particular scene and usually this involves matching the pixel images generated by a model to those in a digitized map or remotely sensed image, but—and this is important—ignoring the configurations of those elements in relation to each other (Torrens, 2006a). Pixels (picture elements) in one scene are simply registered to another scene and the level of coincidence between the two is gauged.

The most straightforward approach to pixel matching is to fashion an inventory of pixel attributes within a simulated scene and to compare the results to corresponding attributes in a remotely sensed image. In analyzing output from their models, Clarke and colleagues (Clarke et al., 1997) collated information regarding the total number of urban pixels (urban extent), the number of edge pixels on the boundary of a simulated landscape, and the amount of pixel clusters at various stages in the course of a simulation run. They then performed a validation exercise by determining the correlation between those results and observed "knowns" from historical maps of the area. Pixel matching can also be performed on a pixel-by-pixel basis. These techniques originate in image processing, where they are used to evaluate classification accuracy. Coincidence matrices are commonly used to register cell-by-cell comparisons between simulated and remotely sensed scenes: pixels are evaluated to determine whether they are identical on both scenes, in terms of states. In some instances, error data is also calculated. Mismatches may be recorded, and moving filters can be used to discern displacement in the mismatch. There is a problem, however, with spatial autocorrelation (Moran, 1950), that weakens the reliability of correlation statistics of this form when applied over geographically-coincident pixels, and with serial autocorrelation when matching is performed between temporal snapshots (Berry, 1993). Similarly, results at one scale of observation or matching may not hold at other scales (Qi and Wu, 1996).

The kappa-statistic is commonly used in conjunction with pixel matching coincidence matrices. Low values of kappa indicate conditions in which there is little correspondence between observed and expected scenes; high values indicate a "good" match between the two. The kappa-statistic has been used in these contexts in a number of urban cellular automata models (White et al., 1997, Wu, 1998), but there are some important complications associated with the technique. The statistic is almost unsuitably sensitive. If a simulated scene is similar to an observed scene, but the correspondence is mismatched by just one pixel in a few places, the overall accuracy of the match may suffer considerably (Wu, 1998). Dislocation of this variety may be particularly problematic in sparsely-populated areas of a scene (Wu and Webster, 1998). Correspondence between observed and expected results may be highly susceptible to variation when different resolutions are used. Coarse resolutions essentially "average out" disagreement between scenes. In the context of urban models, there may be difficulties associated with particular state variables. States designed to represent transport infrastructure are an excellent example. White and colleagues (1997) noted a displacement—of one cell in value—owing to the rasterization of road and rail in their model. This may seem minor, but it ended up becoming (statistically) significant in the context of coincidence matrices. Moreover, the problem, in this example, was transport-specific, and therefore introduced error to a significant feature of the simulation by misrepresenting transport land-use specifically.

Feature and Pattern Recognition

Recognition exercises focus on identifying particular (and theoretically well-understood and/or significant) features and patterns within model output. An advantage of pattern generation in urban simulations is that the patterns to be sought are often robust to changes in rules and parameter values (Andersson et al., 2002). Whereas pixel-matching techniques deal with relatively simple compositional correspondence between scenes, pattern recognition techniques are used to measure specific (space-time) structures in model output.

For example, edge detection may be used to measure the morphology of urban boundaries: the perimeter of an entire city, or the boundary of zones of activity within a city, or well-understood morphologies such as downtown, suburbs, exurbs, and urban-rural fringe (Torrens, 2008). Fractal analysis (Batty and Longley, 1994) can be employed in determining space-filling of urban (or landscape) processes and this has the advantage of being quantifiable across model variables and can help in avoiding thorny scale issues. Cluster-frequency spectra may be used to compare hierarchies in urban clustering, to look at central-place structures, for example. White and colleagues (1997) have performed extensive analysis of their models using these techniques, as have Batty and Xie (Xie, 1996). A similar approach is employed by Torrens (2006b) in modeling suburbanization within the American Midwestern Megaloplois, where clustering-frequency is used to distinguish between the varying growth trajectories of cities within that urban system.

Another approach to pattern-based validation is to study urban "patchiness". In landscape ecology (Forman and Gordon, 1986), a patch is representative of a spatial object (with homogenous characteristics or states) situated within a broader landscape, e.g., the coverage of a particular vegetative type within a larger forest composed of several vegetative species. One can easily see how this concept might be related to urban contexts: we could distinguish clusters of retail activity amidst a sea of urban development, "ecologically", for example. There is a variety of spatial analysis techniques associated with landscape ecology, each designed to support the quantification of composition and configuration properties of patches in landscapes (Gustafson, 1998). Several such landscape metrics have been used to validate urban automata models. Goldstein and colleagues (2004), for example, have calculated a variety of spatial metrics to explore the robustness of their SLEUTH simulation of the Santa Barbara region. These metrics are also employed by Torrens in exploring the results of his automata simulations (Torrens, 2006b), as well as in measuring patterns of sprawl in real-world contexts (Torrens, 2008).

Fuzzy pattern recognition directly addresses the weaknesses of pixel-matching techniques, by introducing additional functionality. First, maps, or images that are being registered for agreement are processed to yield “soft”, fuzzy or transitional, boundaries between pixels, rather than the “hard”, crisp, discrete boundaries used in basic matching methodologies (Heikkila et al., 2003). Second, “fuzzy logic” (Kosko, 1993) is used to determine the agreement between scenes, using AI-inspired pattern recognition rather than brute force matching. In addition to determining the *overall* agreement between scenes, steps are added to the procedure to determine *localized* agreement (Liu and Phinn, 2003), using, for example, linguistic membership functions. Power and colleagues (2000) have used fuzzy validation procedures, in this context, to assess the performance of automata models developed by Engelen and colleagues (1995), enabling disagreement between observed and expected scenes to be broken down into state-specific (land-use types) details. This has obvious advantages, beyond remedying the weaknesses of brute-force pixel-matching; it could, for example, highlight whether particular state variables were subject to systematic agreement errors (which could point to data problems or could indicate areas where amendments to a model’s rules might be appropriate).

Running Models Exhaustively

Sweeping the parameter space of a model involves exploring the complete range of outcomes possible with a particular model specification, or looking at its “space of possibilities” (Couclelis, 1997). One approach is to map those possibilities using graphs. Finite state transition graphs can be used to examine the *global evolution*—step-by-step or transition-by-transition—of an automata simulation, relying on graphs (networks) to plot the “state space’ of an automaton (Wolfram, 1994). Essentially, the complete trajectory of a model can be visualized. Early inroads are being made toward such a scheme, beginning with data-mining procedures for automata models (Hu and Xie, 2006).

Using stochastic (probabilistic) constraint parameters creates an interesting problem: different results can be produced from identical parameterizations; there are often a near infinite number of micro-states that might determine macro-conditions, even for a small set of model parameterizations (Oreskes et al., 1994, Wilson, 1970). One way to “smooth out” this sort of variation and to narrow the candidate configurations to a more manageable set size is to employ Monte Carlo Averaging. Simulations can be run from identical conditions or using the same parameter values (variation then comes from different random number draws used in simulation); they may also be run repeatedly, using different combinations of parameter values (Li and Yeh, 2000), or using variable start conditions. Monte Carlo Averaging is also useful for generating probability maps for use in prediction. Simulations with the SLEUTH model, for example, have been run using Monte Carlo Averaging in an application to the Santa Barbara Region, enabling the selection of locations based on a cut-off rate of 90% success (Goldstein et al., 2004).

CONCLUSIONS

This chapter has presented a review and discussion of the state-of-the-art in calibration and validation of automata models to urbanization applications in the context of complex and dynamic city-systems. A variety of techniques have been introduced and assessed. It is important to realize, however, that many of the models described in this chapter are in very early stages of development. Also, in the context of calibration and validation, it is noteworthy that the intentions of many of the modeling projects and exercises discussed here differ from those that characterize work in land-use and transport modeling traditions common in support of municipal planning. Automata modeling represents somewhat of a paradigm shift in urban simulation (Albrecht, 2005), away from thinking of models as diagnostic or prescriptive tools, toward a conceptualization of urban models as artificial laboratories for experimenting with ideas about urban dynamics. Consequently, many models may not be validated at all; they may be developed as pedagogic instruments, or as “tools to think with”. Accordingly, we might consider a broad spectrum of models (Torrens and O'Sullivan, 2001), ranging from very simply-parameterized models in the tradition of Wolfram’s CA designed to test universality (Wolfram, 1984) to “fuller” planning support systems designed to assist planning management, and policy exercises (Torrens, 2002, Engelen et al., 2002). Depending on their position on this spectrum, models may have different calibration and validation requirements.

Nevertheless, there are some important issues that relate to calibration and validation across that spectrum, including simplicity in model specification, data issues, the generality of models, and the relationship between models and urban theory. Simplicity is one of the most commonly advertised advantages of automata models. This stems from their association with the idea of generative emergence—the concept that simple rules can generate surprising and intricate complexity and that, unlike chaos, the path from simplicity to complexity can be traced through a causal relationship (Batty and Torrens, 2005). Those ideas are often taken at face value when automata models are developed: simple parameters are often introduced to models—and choice may be a function of what data are to hand—and simulations are run as "blue skies" experiments to see, essentially, what will come out. A problem with using automata in this regard is that as simulations runs evolve beyond initial conditions, automata (and particularly urban cellular automata) have a strong tendency to "go exponential" and must often be tightly constrained in order to produce patterns that resemble real cities. The resulting "soup" is sometimes confused with emergent phenomena (Epstein, 1999, Faith, 1998).

Another issue relates to the role of automata modeling in the experimental process. Urban automata models are often borrowed from the physical sciences; while automata methodologies are usually similar regardless of application (an automaton is an automaton after all), but, urban automata *experiments* often bear little resemblance to those in fields such as computer science, physics, and chemistry (Oreskes et al., 1994), where experiments deal with systems that are relatively well-understood in comparison to urban systems. The idea of simple models generating surprising complexity is a powerful one, but is predicated on the notion that an (often small) set of the "right" rules are out there, that the simple ingredients to a complex system can be uncovered. As Wolfram wrote, a model developer should, "attempt to distill the mathematical essence of the process by which complex behavior is generated. … To discover and analyze the mathematical basis for the generation of complexity, one must identify simple mathematical systems that capture the essence of the process" (Wolfram, 1994) (p.411). These sorts of sentiment are wonderfully romantic in their tractability and parsimony. Alas, the reality is quite different: indeed, Wolfram spent the next two decades searching for sets of simple rules (Wolfram, 2002) and many believe the issue to be a red herring (Horgan, 1995). Of course, in the context of urban systems, we often have no idea what the "right" rules are (if we did, planning cities would be easy). The rules are always changing and there are myriad confounding influences on any given urban process. Nevertheless, urban automata models can be used as exploratory tools, experiments for evaluating what the "right" rules might actually be, what dynamics might result given a particular set of candidates for the "right" rules, or where we might efficiently devote our intellectual efforts in searching for them. Recent emphasis in the literature on calibration and validation is certainly taking the field in that direction and provides opportunities for it to evolve from early, experimental phases.

Validation and calibration verification exercises are inextricably intertwined with data. This relationship can be synergetic in some cases, and terribly constraining in others. One criticism that could be made of several of the parameter-based calibration mechanisms that I have discussed in this chapter is that they are data-specific; models may become "captives of their data sets" (Ward et al., 2000b). Also, many automata models require individual-scale data, of individual households, parcels of land, and so on. Some detailed models have been developed where model developers have access to entity-scale databases (Benenson et al., 2002), but such data may not always be available. A confounding issue is that calibration and validation with data from particular locations may result in a model that is "fit" for use in that location, but is not applicable to other cities or times. The danger is that, after careful calibration and validation, you may end up, not with a model of sprawl, for example, but with a model of "sprawl in Bloomington, Indiana.

A way to dodge this problem is to design urban automata models for general use, with general rules of urbanization that transcend the specifics of a particular location, problem, or period. The models developed by Roger White, Guy Engelen, and colleagues at the Research Institute for Knowledge Systems (RIKS) are a good example of this approach; the models have been applied to a diverse range of scenarios in various locations, including the Netherlands, Saint Lucia, Dublin, and Cincinnati (Engelen et al., 1995, Engelen et al., 2002, Power et al., 2000, White, 1998, White and Engelen, 1993, White and Engelen, 1994, White and

Engelen, 1997, White and Engelen, 2000, White et al., 1997). Keith Clarke's SLEUTH model has also seen a rich range of applications. It has been used to model urbanization in the Santa Barbara, the San Francisco Bay Area, Washington D.C. and Baltimore, Lisbon, and Porto (Herold, 2002, Goldstein et al., 2004, Candau et al., 2000, Silva and Clarke, 2002, Clarke, 1997, Clarke and Gaydos, 1998, Clarke et al., 1997). In addition, Benenson and colleagues at Tel Aviv University's Environmental Simulation Laboratory have developed a general all-purpose modeling environment (Benenson et al., 2006) for building simulations of *any* description, based on the idea of reconfigurable and malleable Geographic Automata Systems (Torrens and Benenson, 2005). However, general models lose some fidelity to detail, almost by definition, and how to reconcile more specific models in this sort of ecosystem is a question that remains to be answered.

Ultimately, several of these issues discussed above relate to a central concern: the relationship between models and theory. Models can be calibrated with vast quantities of detailed data, and using sophisticated procedures. They can be validated for historical time periods with high degrees of success. However, a model is only as good as the rules that drive its behavior. Good rules require good theory. The relationship is symbiotic: good theory often relies on good models to test the theory. Interestingly, the emergence of automata models has facilitated the exploration of new question about urban systems, and the evaluation of hypotheses that were hitherto inaccessible with conventional simulation methodology (Batty, 2005). But, in many instances, theory has been found wanting, particularly at micro-scales and in relation to phenomena that operate across scales. Conventional simulation methodology is inadequate, in many respects, for exploring ideas about urban dynamics in terms of complex adaptive systems. Nevertheless, these issues were present in previous generations of urban models and remain unresolved. While still in its relative infancy as a field, automata models, with their almost limitless malleability, are the best option we have for reconciling theory, plans, and reality through simulation.

ACKNOWLEDGEMENTS

This material is based upon work supported by the National Science Foundation under Grant Nos. 1002519 and 0643322.

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