

Sensitivity analysis of a cellular automata land use model through multiple metrics of goodness-of-fit

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Abstract: The complexity and self-organizing behaviour of Cellular Automata models makes them attractive instruments for investigating urban change processes. That same complexity, however, obscures the relation between model parameters and model results and poses problems for the calibration of the models as well as the interpretation of results. This paper introduces an approach to sensitivity analysis that untangles much of the complex relation between parameters and outputs. The key of the approach is to find compartments in parameter space on the basis of the relation between multiple metrics of goodness-of-fit. Within individual compartments the relation between parameters and model outputs is less chaotic and open for investigation by more traditional means. The method offers prospects for model calibration and parameter reduction; further steps in these directions are outlined and discussed.

1. INTRODUCTION

Cellular automata (CA) models have become widely used for simulating land use dynamics. This type of model has found is used to test hypotheses about urban change processes and to investigate landscape scale

consequences of local interactions and behaviour (Batty, 2005). In urban planning practice, CA models have become the foundation of planning support systems that allow spatial planners to explore the consequences of different plans and policies and the robustness of these under different scenarios or degrees of uncertainty.

CA models of land use dynamics represent space by means of a regular grid (raster). Each of the cells in the grid has a particular state, which is a land use class such as 'residential', 'commercial' or 'industrial'. The states of the cells change in time on the basis of transition rules, which are based on cells in the neighbourhood. For instance a transition rule may prescribe that a cell of 'residential' is likely to become 'commercial' if it is bordering another 'commercial' cell and is otherwise surrounded by 'residential' cells.

One alluring characteristic of CA models is that the interaction and feedbacks between neighbouring cells can give rise to the kind of chaotic dynamics that also characterize real urban systems. Relatively simple spatial interaction rules demonstrate to be very plausible explanations for the complex urban morphology as it can be observed.

Attractive as it is, the CA mechanisms also presents challenges to spatial analysts; like all models, CA only behave according to their specifications. Nevertheless, the complex and self-organizing character of the models obscures the relation between parameter settings and model behaviour. It is not always clear why the models produce certain morphological patterns. This limits the degree to which lessons about the relation between pattern and process can be drawn from CA. It presents practical problems when determining the right or optimal parameter values for CA models.

Even when the model takes no parameters, the CA formulism requires at least the meta-parameters of cell size, time step and neighbourhood size. Consequently, sensitivity analysis is useful - if not required - for any CA modelling exercise (Kocabas and Dragicevic, 2006).

This paper presents an approach to sensitivity analysis that incorporates recent developments in spatial analytical techniques to measure the agreement between model and reality from different perspectives. The map comparison methods address model agreement at different scales and consider both aspects of presence and structure (Hagen-Zanker and Martens 2008). By incorporating such diverse metrics, the sensitivity analysis is expected to provide insight in a broad range of behaviour of the model. By focussing on agreement between model and reality, this paper intends to steer the sensitivity analysis to those regions in parameter space that bear a relevance to reality and ignore the model particularities of regions in parameter space that are not realistic anyway. After all, the ultimate objective in the end is to learn about urban systems and not about CA models.

In his paper a highly reduced version of the Constrained Cellular Automata (CCA) (White, Engelen, et al., 1997) is evaluated over a wide range of parameter values. For each set of parameters the model is run for a period in the past and the final map of the simulation is compared to the actual map at the end of the simulation period according to multiple goodness-of-fit metrics. The experiment produces a full series of goodness-of-fit metrics for each combination of parameters. Cluster analysis on this data set is the foundation for the sensitivity analysis presented in this paper.

The paper is organized as follows: Section 2 introduces the CA model, the goodness-of-fit metrics. Section 3 presents the application case and the results of the sensitivity analysis. Finally, section 4 discusses the results and conclusions including a recommendation for a calibration procedure for this kind of models that follows from the interpretation of the results.

2. METHOD

2.1 Reduced CCA land use model

The model that is applied is a Constraint Cellular Automata as it is introduced by (White, Engelen, et al., 1997). The model is highly simplified compared to other applications of the model (de Nijs, de Niet, et al., 2004; Barredo and Demicheli, 2003; Engelen, White, et al., 2003) since it only knows 2 land use types; urban and non-urban of which non-urban is only modelled passively. In other words, the transition rules only determine which cells become urban and the remaining cells are non-urban.

A further simplification concerns the additional data layers of the model that determine the transition potential of a cell. In these applications, other layers beside the neighbourhood determine the transitions. These are accessibility, suitability, zoning status and a random perturbation. Of these layers only the random perturbation is retained in the model applied here.

What remains is a model in which an exogenous claim for urban area is on a year by year base allocated on the basis of a transition potential for urban area. The transition potential of a cell is a function of the land use types found in the neighbourhood and the random perturbation factor. The transition potential is calculated according to the following equations:

$$P_x = N_x R_x$$

Where P_x is the transition potential at location (cell) x . N_x is the neighbourhood component of the potential and R_x is the random perturbation. The neighbourhood component is defined as follows:

$$N_x = \sum_{y=0}^{nbh} w(L_{x,y}, d_{x,y}) \quad 2$$

Where y iterates over all cells in the neighbourhood of x . $L_{x,y}$ is the land use class found at the y -th neighbour of x and $d_{x,y}$ is the distance between cell x and neighbour y . $w(l,d)$ is the contribution of land use class l to the potential from distance d . The weight function is determined as follows:

$$w(L,d) = \begin{cases} \text{if } L = \text{urban and } d = 0 & \infty \\ \text{if } L = \text{urban and } d = 1 & c_1 + nb \\ \text{if } L = \text{urban and } d > 1 & c_1 * 0.5^{\frac{d}{h_1}} \\ \text{if } L \neq \text{urban and } d = 0 & 0 \\ \text{if } L \neq \text{urban and } d > 0 & 0.5^{\frac{d}{h_2}} \end{cases} \quad 3$$

Where c_1 , h_1 , h_2 , and nb are parameters. This particular function was devised to have a large flexibility with the extent to which urban areas are attracted to urban or non urban. The parameter c_1 determines whether at short distances urban or non-urban is most attractive; above 1 is urban and below 1 is non-urban. At larger distances this is not only determined by c_1 but also by the distance decay of the impact of both urban and non-urban (halving distances h_1 and h_2). The factor nb is added to the first neighbour from the consideration that new urban area developed adjacent to existing urban area can benefit from the infrastructure already present. nb can thus be described as the infrastructure bonus. The weight function at distance 0 is determined such that only the transition from non-urban to urban takes place and not the reverse. Figure 1 illustrates the weight function.

The degree of stochasticity is also parameterized, using the equation proposed by (White, Engelen, et al., 1997).

$$R_x = 1 - \ln(\alpha * U_x) \quad 4$$

where U_x is a random number from a uniform distribution between 0 and 1. A new number is drawn for each cell and each time step. α is a parameter that determines the degree of noisiness. This particular distribution produces few, but strong outliers.

The total area of urban land (the land claim) in each time step is exogenously determined. The cells with the highest potential become urban, the others remain non-urban.

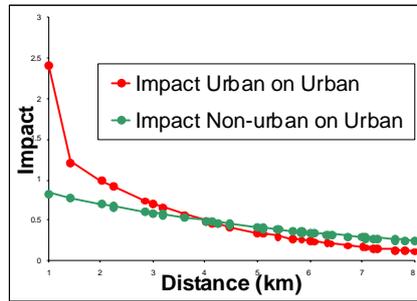


Figure 1 The neighbourhood functions

The reason for simplifying the model to such a great extent is to allow a brute force sensitivity analysis that includes all parameters. 5 different values were pre-selected yielding $5^5 = 3125$ different parameter combination as shown in table 1.

Table 1 Parameter values for the brute force sensitivity analysis

	#1	#2	#3	#4	#5
α	0	0.01	0.02	0.03	0.04
c1	0	1	2	3	4
h1	0.25	0.5	1	2	4
h2	0.25	0.5	1	2	4
nb	0	1	2	3	4

A brute force sensitivity analysis entails running the model once for all parameter settings and calculating the goodness-of-fit for each run according to different metrics (described in the following section). The fact that the model is stochastic in nature and outcomes will vary run to run is not accounted for.

2.2 Goodness-of-fit metrics

In recent years a multitude of methods has been developed for the evaluation of raster based simulation model on the basis of map comparison. Hagen-Zanker and Martens (2008) present an overview of methods and

propose a framework to classify different methods. The framework classifies map comparison methods according to two attributes.

The first distinguishing attribute is the spatial scope of the units that are analysed. Local, focal and global comparison methods are distinguished. Local methods are also called cell-by-cell methods. Focal methods apply a moving window and the agreement associated to each location is that pertaining to the window around that location. By applying focal methods with different window sizes a multi-scale analysis is established. Global comparison metrics evaluate the agreement of global attributes of both maps, for instance the fractal dimension.

The second attribute that differentiates comparison methods is whether they address agreement in terms of the presence of the mapped variable or its spatial configuration. Local comparisons never consider spatial configuration, simply because at the level of a single cell it is not possible recognize any aspect of configuration. At the global level, only configuration metrics will be evaluated because the global presence of each land use category is an endogenous input to the model and will therefore be identical in all model runs.

An overview of goodness-of-fit metrics evaluated in this paper is presented in table 2.

Table 2 Goodness-of-fit metrics

Metric	Scope	Attribute	Main reference
Kappa	local	presence	Monserud and Leemans 1992
Fuzzy Kappa	focal	(near) presence	Hagen 2003
MW Patch size	focal	structure	Hagen-Zanker 2006
MW Fractal dimension	focal	structure	Hagen-Zanker 2006
GL Patch size	global	structure	Turner et al. 1989
GL Fractal dimension	global	structure	Turner et al. 1989

MW = moving windows based, GL = global

2.2.1 Local presence: Kappa

A highly intuitive method of comparing two land use maps is to calculate the fraction of all cells where both maps are identical. The fraction correct that follows from this analysis has a disadvantage however; it tends to consider maps where one or a few land use classes dominate more similar. For instance, take the case where two maps are compared that both are covered for 80% by the category 'desert'. It follows logically that at least 60% of the map consists of cells that are 'desert' in both maps; the expected fraction of cells that is desert in both instances is 64%. The Kappa (Cohen 1960, Monserud and Leemans 1992) corrects for this expected agreement

and returns a value between -1 (full disagreement) and 1 (perfect agreement, whereby the value 0 corresponds to the expected agreement).

2.2.2 Focal presence: Fuzzy Kappa

The Kappa statistics is a metric for the comparison of paired observations. It is not strictly speaking a map comparison method because it does not consider spatial relations except cell-to-cell overlap. The fuzzy set map comparison (Hagen, 2003; Hagen-Zanker, Straatman, et al., 2005) offers an extension to the Kappa statistic that not only registers cell-by-cell overlap, but also gives credit for near cell-by-cell overlap.

Fuzziness of location introduces a locational tolerance to the effect that cells that are not taken in by the same land use class may still be considered similar to a degree if matching categories are found in the proximity. A two-way comparison is applied, meaning that for the category found in the first map a counterpart needs to be found in the second map and vice versa. The smallest distance within which a matching cell is found in both neighbourhoods determines the similarity of the location. The value of the similarity is found by means of a distance decay function as follows:

$$S_x^{A,B} = 0.5^{\min(nn_x(A,B), nn_x(B,A))/h} \quad 5$$

where $S_x^{A,B}$ is the similarity of map A and B at location x . The function $nn_x(A,B)$ gives the nearest neighbour distance in map A at location x to the land use class found in map B at location x . The parameter h is the halving distance and determines the degree of spatial fuzziness. Note that this notation is a simplification compared to (Hagen-Zanker, Straatman, et al., 2005) that can only be made since fuzziness of category is not considered in the current case.

Like the Kappa statistic, the Fuzzy Kappa statistic corrects the fuzzy fraction of agreement for the expected fuzzy fraction of agreement. Perfectly agreeing cells have value 1 and the random expected agreement is 0. It is possible however to find Fuzzy Kappa values below -1. If the degree of fuzziness is minimal, then Fuzzy Kappa is identical to Kappa.

2.2.3 Focal structure: Patch size and fractal dimension

One of the strengths of cellular automata models is that they capture the processes underlying the formation of urban morphology. As the growth of urban areas can be chaotic and is hard or impossible to predict, it may be more appropriate to measure model performance in terms of spatial structure

than in (near) location-to-location overlap. (Hagen-Zanker, 2006) introduces several methods on the basis of moving windows that evaluate structural similarity at multiple scales. The map comparison methods are based on structure metrics more commonly used in landscape ecological applications and are generally available in the FRAGSTATS software (McGarical, Cushman, et al., 2002). The extension of (Hagen-Zanker, 2006) is to calculate the pattern metric not for the whole map, but for a window surrounding each location. The difference in structure between two maps is then calculated on the basis of a window by window comparison.

The focal structure comparisons that are applied in the current paper are based on urban patches (or clusters), which are contiguous areas of the land use class urban. Two characteristics of these clusters are measured their size (measured as the number of cells) and their shape complexity. The complexity of the shape is measured by means of the fractal dimension using the following equation:

$$F_c = \frac{2 * \log\left(\frac{1}{4} P_c\right)}{\log(A_c)} \quad 6$$

Where F_c is the fractal dimension of a patch, P_c is the perimeter and A_c is the area. Area and perimeter are measured in cell units. The fractal dimension ranges from 1 for simple shapes to 2 for complex shapes. A moving window is applied to calculate a mean fractal dimension for every cell on the map, using the following equation:

$$f_x = \frac{\sum_{i=1}^{n_x} w_i * F_{c_i}}{\sum_{i=1}^{n_x} w_i} \quad 7$$

Where f_x is the mean fractal dimension of the window centred on the cell x . The index i iterates over all cells in the window around x . n_x is the number of cells in the window centred on x . F_{c_i} is the fractal dimension corresponding to the patch that contains the i -th neighbour of cell x and w_i is the weight pertaining to that cell. The weight is determined such that cells of the class urban are considered and the total weight for each urban patch is 1:

$$w_i = \begin{cases} 1/S_{c_i}, & \text{if } L_i = \text{urban} \\ 0, & \text{else} \end{cases} \quad 8$$

Where S_{ci} is the patch size of the patch containing cell i and L_i is the land use class found at cell i .

The mean patch size of the window centred on a cell is calculated analogous to the mean fractal dimension. The moving window based structure maps (patch size and fractal dimension) are compared on a root mean squared basis:

$$d_f^{A,B} = \sqrt{\sum_x (f_x^A - f_x^B)^2}$$

$$d_s^{A,B} = \sqrt{\sum_x (s_x^A - s_x^B)^2}$$

Where $d_f^{A,B}$ is the difference between map A and B in terms of the moving window based fractal dimension. Likewise $d_s^{A,B}$ is the difference in moving window based patch size. f_x^A is the mean fractal dimension at cell x in map A (likewise for B). s_x^A is the mean patch size at cell x in map A (likewise for B).

2.2.4 Global structure: Patch size and fractal dimension

At the focal level patch size and fractal dimension are evaluated using a moving window, as the previous section explains. These metrics are also calculated for the whole study area, whereby they summarize global structure in a single value. This is the approach followed by (Turner, Costanza, et al., 1989).

3. APPLICATION & RESULTS

The model is applied for Portugal on the basis of the CORINE dataset (Haynes-Young and Weber, 2006) aggregated to represent the country at 1 km resolution and by two classes urban and non-urban. The data is available for two years: 1986 and 2000. Over this period, the model takes 10 time steps. Figure 2 shows the map of 1986 which is used to run the model and the map of 2000 which is used to evaluate the model.

For the sensitivity analysis the model is run 3125 times under different parameter settings. Figure 3 presents some assorted outputs of these runs to illustrate the variance that is present within the investigated parameter space. The goodness-of-fit metrics evaluate different parameter sets as having the best fit. Figure 4 shows different ‘best fits’ according to all metrics.

Since the different goodness-of-fit metrics do not agree on the best fitting parameter set, it becomes interesting to investigate the relationship between the different goodness-of-fit measures. These relationships are visualized on the basis of scatter plots. These plots are presented in figure 5.

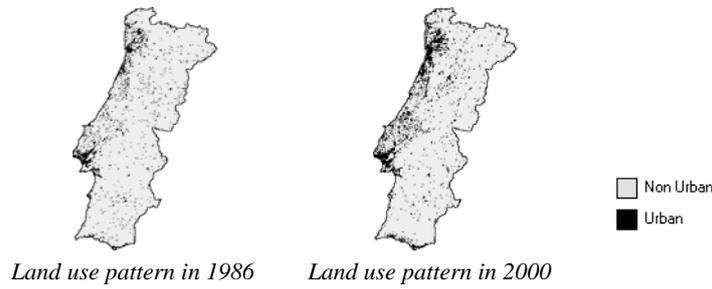


Figure 2 CORINE land use maps of Portugal, spatially aggregated to 1 km² cells and thematically aggregated to two classes: urban and non-urban



Figure 3 These outputs of the model under assorted parameter settings illustrate the variability present within the parameter space

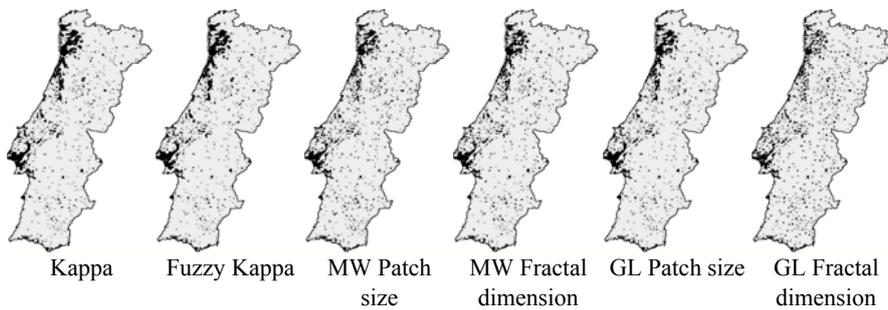


Figure 4 Best fitting model results according to 6 goodness-of-fit metrics

Figure 6 again shows the scatter plot with the most pronounced cluster, which is the plot of fuzzy kappa and global fractal dimension. 8 clusters are identified (C0 to C7) and each is typified by a (near) linear relation between fuzzy kappa and fractal dimension.

Cluster C0 consists of some runs with very poor performance in terms of fuzzy kappa. Cluster C2 and C3 are not of much interest, since the goodness-of-fit, both in terms of fuzzy kappa and fractal dimension is relatively low. It is noteworthy however that C2 represents a group of parameter settings that is variable in fractal dimension, but not in fuzzy kappa. C3 presents the opposite, parameter settings that vary in fuzzy kappa but not in fractal dimension. Cluster C5 has a similar pattern, yet a better fit in terms of fuzzy kappa.

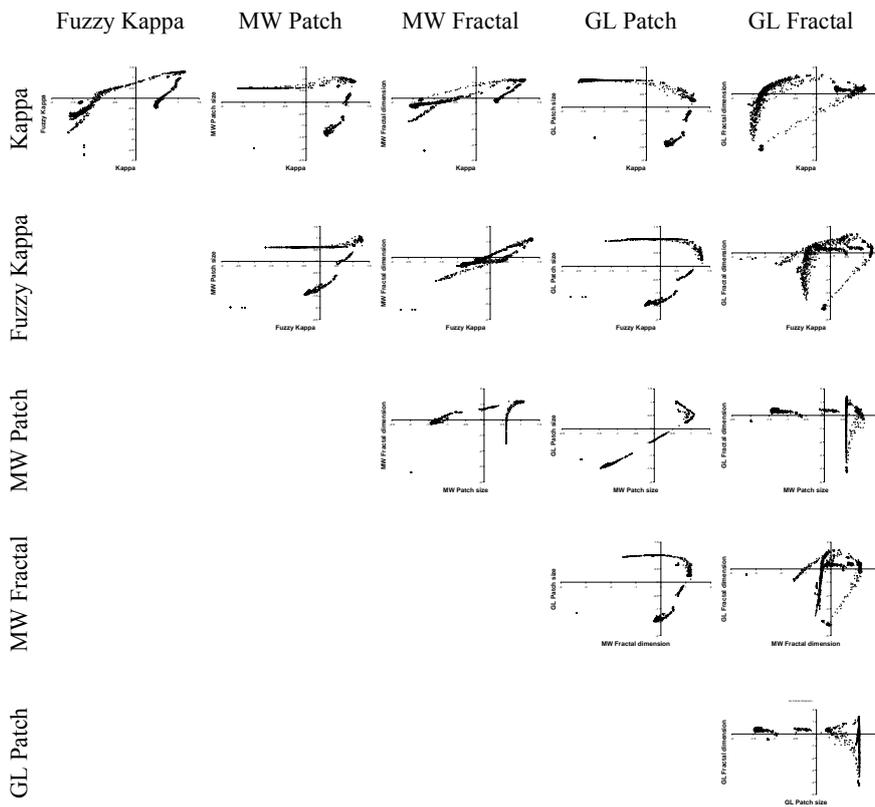


Figure 5 The scatter plots of the results from 3125 parameter sets according to different pairs of goodness-of-fit metrics reveals a strong clusters.

Of most interest are clusters C1, C6 and C7 because these include the upper ranges of goodness-of-fit according to both metrics. Both C1 and C7 have a positive relation between the two goodness-of-fit measures, meaning that an increase in one metric is associated with an increase in the other. Regrettably, these clusters do not extend indefinitely or to the maximum

level of agreement. Instead, at one point parameter settings fall within cluster C6 where a trade-off between goodness-of-fit according to both methods takes place.

The identified cluster can be related back to the parameter values. For instance all parameter settings where h_1 is equal to h_2 lie within either C6 or C7. In almost all parameter settings of cluster C1, h_1 is smaller than h_2 .

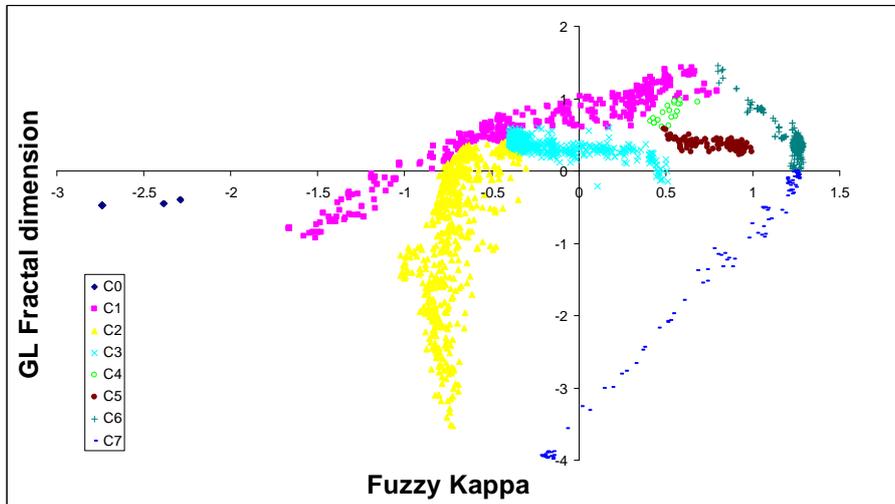


Figure 6 Seven clusters identified in the relationship between Fuzzy Kappa and Global Fractal Dimension

4. DISCUSSION AND CONCLUSION

Analysis of the results reveals a strong clustering. Strikingly, the different clusters are not centred on particular goodness of fit levels. Instead the clusters can be described as a small number of linear functions with a specific range and domain. The interpretation of this result is that the different clusters represent parameter settings that correspond to a spatial process (e.g. clumping versus scattering or growth in rural versus urban areas). The place of a parameter combination within the cluster may determine the strength of the process.

This interpretation would also explain the fact that in many cases pairs of clusters describe a turning point, for instance clusters C6 and C7 in figure 6. These clusters may be interpreted as cases where one cluster represents a particular process too strongly and the other cluster represents the same process too weakly.

It must be noted though, that although in the current case 8 clusters have been identified, it did not become clear which processes underlie these clusters. The relatively simple pattern of focal patch size plotted against global patch size suggests that the balance between patch growth and patch formation is one of the processes underlying the clustering. Even though a more detailed analysis of the processes underlying the clusters would be feasible, that analysis is not part of the study, because it cannot be expected that such analysis would still be possible when a 'normal' non-simplified Constrained Cellular Automata model is considered.

The insight gained into the behaviour of the model under different parameter setting offers interesting opportunities for the calibration of cellular automata land use models or spatial dynamic models in general. The calibration of CA models is a well known problem (Straatman, White, et al., 2004), especially because of the non-linear relationship between parameter values and goodness-of-fit. The sensitivity analysis and subsequent cluster analysis presented here can simplify the problem. Regions within parameter space can be identified within which the complexity of the model is greatly reduced (witness the linear relation between goodness-of-fit metrics) and conventional methods such as hill-climbing and line-search can be applied. Furthermore, it is not necessary to investigate all clusters that are identified. From the relationship between goodness-of-fit measures it is possible to identify those clusters with prospects of containing a optimum fit.

This interpretation of the results suggests a calibration procedure that takes the following steps:

1. Sample parameter space randomly or structurally
2. Identify clusters of parameter settings using an unsupervised classification for clusters of points along lines in the n -dimensional space of goodness-of-fit metrics. For instance applying the algorithm of (Chou, Lin, et al., 1999)
3. Identify clusters of parameter values using a supervised classification on the basis of the clusters found in the previous step. For instance using decision tree induction (Quinlan, 1986).
4. Remove from parameter space those parameter settings that lie within clusters along which lines no optimal fit can be found.
5. Apply conventional optimization methods (hill-climbing, line-search) to find the optimal parameter settings within the clusters that lie along lines that may include the optimal fit

The results, especially the variation in the landscape of optimal fit in figure 4, confirm earlier conclusions (Hagen-Zanker 2006, Hagen-Zanker and Martens 2008) stipulating the need of assessing spatial models according

to multiple criteria. When confronting the maps of figure 4 with the author's subjective visual assessment, the Kappa and Fuzzy Kappa steer towards landscapes that are too clumpy. The global fractal dimension on the other hand finds an optimal fit that is a 'fringe' solution; urban growth is found at completely wrong locations, but by accident the resulting fractal dimension is similar to that of reality.

Another application of these results is in the reduction of the number of parameters in the model. In the original CCA model (White, Engelen, et al., 1997) the number of parameters describing the neighbourhood effect from one land use type onto another is 30. In the current case this has been reduced to maximally 3 (*h1*, *c1*, *nb*). This reduction however is based on personal experience and preference and therefore rather arbitrary. The proposed procedure, whereby the parameter space is partitioned on the basis of clusters found in the relation between goodness-of-fit measures, can be a guide in selecting appropriate parameter generalizations. Attractive generalizations would be those where the reduced parameter settings form the same clusters as the full parameter set, at least in the ranges where the model performs relatively well. A second criterion would be that attractive generalizations are those where the relation between parameter values and cluster is most straightforward.

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