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The Future of Central European Cities – Optimization of a Cellular Automaton for the Spatially Explicit Prediction of Urban Sprawl

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Abstract

The quantitative and qualitative measurement, prediction and evaluation of urban sprawl have come to play a central role in land-system science. One of the most important and most implemented artificial intelligence (AI) techniques in terms of urban systems simulation is cellular automata (CA) like SLEUTH. SLEUTH models the physical urban expansion by accomplishing four simple growth rules with every modeling step. Simultaneously, SLEUTH also reflects main drawbacks of CA since they contain a higher degree of stochastic variation leading to a simulation uncertainty. This chapter will explain how the simulation power of CA can be optimized by combining them with the machine learning algorithm support vector machines (SVMs). Conceptually in SVMs, input vectors are projected in a higher-dimensional feature space in which an optimal separating hyperplane can be constructed for separating the input data into two or more classes. In the comparative analysis, the integrated modeling approach is carried out for a unique postindustrial European agglomeration: The Ruhr Area. It will be demonstrated how the AI learning approach is implemented, calibrated, validated and applied for the prediction of the regional urban land-cover pattern between 1975 and 2005. Finally, the probability effects will be visualized with the concept of urban DNA.

Keywords: support vector machines, Cellular automata, SLEUTH, urban growth, probability maps

1. Introduction

The American landscape designer Earle Draper initiated a term describing the unaesthetic and uneconomic settlement structure of American cities in his 1937 lecture on town planning. In reflecting the obliteration of rural and urban spaces, this term grew more and more in popularity: “perhaps diffusion is too kind of word. in bursting its bounds, the city actually sprawled and made the countryside ugly, uneconomic [in terms] of services and doubtful social value [1]”. Ever since the term ‘sprawl’ emerged in a geographical context, nearly 80 years have passed and the specific patterns and processes of growing cities have developed from an American to a European problem in general and a German problem in particular [2–5]. Being one of the most challenging land-use and land-cover changes implicating several consequences for the anthropogenic and geobiophysical spheres, urban sprawl has become an inherent part of the international sustainability discourse in the context of global change [6–10]. The same holds true for geographical research with its long history of diverse theories and models of land-use change in general and urban sprawl in specific [11–16]. One of the most important streams of urban models understands urban areas as complex systems. Those geosimulation techniques make use of artificial intelligence (AI) to model the micro processes being responsible for the macro pattern of urban systems [11, 12, 17]. Following the famous quote by Aristotle “the whole is more than the sum of its parts”, they model urban systems in a bottom-up manner. Cellular automata (CA) are very popular geosimulation tools. SLEUTH is a well-known urban CA [18]. It is a purely growth-oriented model and as a bottom-up approach it is not dependent on intensive prestudies about the general causes of urban growth or the location-specific determining factors. Based on the principles of neighborhood effects and spatial autocorrelation, the simulation rules are relatively simple. However, SLEUTH is able to capture complex emergences of urban patterns so that it has been applied in several urban growth studies all over the world [19]. Although the performance of CA for spatially explicit urban land-use simulation is very high, it gives no direct insight into the relationship between nonspatial human and ecological driving forces, spatial determining factors and the emergence of urban growth. The semistatistical method called support vector machines (SVMs) [20] is able to avoid this disadvantage: developed for solving nonlinear classification problems, SVMs are also suitable for analyzing the spatial driving factors of urban land-use change. They are a machine learning concept based on statistical learning theory. The basic idea is to project input vectors on a higher dimensional feature space, in which an optimal separating hyperplane can be constructed for separating the data into two or more classes. By using a specific feature selection, neglectable features can be separated and important features can be identified.

The objective of this contribution is to demonstrate how the simulation skills of CA on the one hand and SVM on the other hand can be integrated in order to achieve an optimized modeling approach. The anchor point for joining AI and machine learning physique is the exclusion layer of SLEUTH. Instead of the standard input map of the CA defining restriction areas where no urbanization is allowed to take place, a probability map derived from SVM will be utilized. In a nutshell, the coupling of SLEUTH and SVM is undertaken in order to answer the following research questions:

1. Which driving factors influence the physical urban growth in the Ruhr and how do they take effect according to a SVM feature selection?
2. Do SVM guide SLEUTH and do they optimize its modeling ability?
3. How well do SVM perform in comparison to standard SLEUTH implementations?

Figure 1. Land-use map (2006) with cities and districts of the Ruhr (North Rhine-Westphalia, Germany) [2].

The main study area which SLEUTH-SVM is set up for lies in the western part of Germany and in the central part of NRW: the Ruhr (**Figure 1**). With a polycentric and administratively fragmented structure but a homogenous and extensive urban area, the Ruhr is a worldwide unique urban entity. In general, 11 cities and 4 districts form the biggest agglomeration (1150 people per km²) in Germany, and with its 443,969 ha it is the fifth largest urban region in Europe. Concerning the geosimulation of urban systems, the Ruhr proves to be suitable due to two principal aspects: Firstly, it exhibits the highest absolute rates of urban sprawl in

Germany. Between 1975 and 2005, the agglomeration grew around 37,022 ha with a total urban area of 94,990 to 132,012 [21]. Compared to other sprawling cities in Germany, the Ruhr's urban expansion can be described as a 'metropolitan suburban sprawl' type with high values of new land consumption and with low fragmentations and dispersion patterns in the core area coexisting with lower densities and patched open spaces in the suburban area [5]. Secondly, the Ruhr acts as a 'hero' in the scientific discourse of demographic decline and structural transformations in old industrialized cities. Like other members of the 'rusty fellowship', the Ruhr has to struggle with archetypical problems of the former monofunctional manufacturing cities depending on mining and heavy engineering: a demographic decline, an aging population, high unemployment rates, an incipient brain drain and a lack of incentives to attract prosperous companies of the service sector, especially the 'new economy' [22, 23]. Before the CA is optimized, a brief overview of the implications of urban sprawl, the complexity of urban systems and important urban models in geography, as well as an introduction into the geosimulation with CA is given.

2. Geosimulation of urban sprawl

2.1. The complexity of urban systems

Urban sprawl is often treated as a specific of urbanization and urban growth. The classification of those processes is not homogenous and their definitions oscillate between the pure expansion of impervious surfaces and the distribution of urban activities and life styles in addition [2, 4, 24]. The study focuses on the land consumption aspects of urban sprawl. That is the conversion from nonurban to urban land cover and land uses for the main part indicating a certain amount of newly built-up, impervious areas [25]. The natural impacts of urban sprawl are manifold and concern several natural spheres. Cities consist by more than 50% of impervious land cover [26]. The sealing of even fruitful and agricultural valuable soils leads to a loss of fertility, transformation, filtering and buffering services [27]. The infiltration is disturbed and the surface runoff can be increased by five times with a sealing fracture of more than 90% [28]. The ecological footprint of a street can be estimated by 2 km and that of a European agglomeration by 1000 times of its area [9]. For a long time, the natural increase of people and migration flows into the cities' core areas as well as the economic expansion of the industrial age constituted the most important factors responsible for the growth of German cities. During the last 50 years, however, the trends of land consumption and population growth have moved apart: While the German population has grown around one fifth, the amount of settlement and traffic areas has nearly doubled [4]. In the literature, the following aspects are mentioned regularly: economic wealth; separation of individuals; the persuasion of the wish for owning a house on greenfield sites; new supply types; demographic change; aging of population; parish-pump politics and dominance of the automobile [2, 29–34]. Those causes build the main underlying driving forces of urban sprawl in Germany. But how do they interact? Which direct impacts do they evoke and what are their spatial outcomes? Why do they induce the emergence of sprawling urban areas even in regions affected by demographic and economic shrinkage?

In order to measure, model and understand urban sprawl, one has to think of it as a kind of urban land-use change embedded in the global land system [35]. The changes of land use and land cover and their driving factors construct nonlinear, complex systems including irrational behavior of their human actors. Therefore, urban areas must be treated as open and dynamic systems in which macro level patterns are a result of behavioral driven processes of micro level [36, 37]. Urban systems exhibit characteristics of hysteresis so that future developments and changes of urban systems are not only influenced by the current environment but also by the past one [32, 38, 39]. The initial configuration of its states affects the future decision making of its actors. Exemplary, road expansions do not only improve the infrastructural development but also change the spatial pattern affecting the circulatory system of a region's economy and feeding back to road improvements [40]. Thus, the observation scales of time (1) and space (2) are fundamental elements for the analysis of urban systems: (1) Technological innovations or new policies are exogenous drivers and affect sprawling urban growth in a short term. Due to coevolutionary interaction between states and actors, they become endogenous and are affected by urban dynamics in a long term [32]. (2) While on an aggregate level, residential areas may be clustered resulting in a positive spatial autocorrelation, and on an individual level, a certain range of distance may be kept resulting in negative spatial autocorrelation [41, 42].

2.2. Geosimulation – Using the AI of cells

The new wave of urban simulation often goes under the name of geosimulation. They shifted the modelling paradigm from macrostatics to microdynamics, from aggregation to disaggregation, from homogeneity to heterogeneity and from equilibrium to disequilibrium in urban modeling. Mandl defines geosimulation as a simulation where the modeled system processes, compartments and applications are spatially characterized and exhibit spatial relations [43]. Benenson and Torrens further comprehend geosimulation as “catch title that can be used to represent a very recent wave of research in geography ... [which] is concerned with the design and construction of object-based high resolution spatial models ... to explore ideas and hypotheses about how spatial systems operate [12]”. The implementation of AI methods for urban simulation purposes was heavily influenced by technical progresses in terms of computation, land-use data acquisition, geographic information systems (GISs), complexity studies, as well as the development and use of AI approaches in natural and social sciences outside of geography [17, 44]. Indeed, “geographers arrived somewhat late to the party” of addressing individual behavior alteration as design strategy of simulation applications [45]. The displacement of equations by code offered the possibility to explain the pattern and processes of complex open system dynamics on multiple organizational levels theoretically and experimentally [46]. Hence, the research object of urban sprawl could leave the suggestions of order, stability, linearity and rationality rooted in general system theory.

One of the most important and most implemented geosimulation techniques in terms of urban systems simulation is CA. The invention of CA is attributed to the mathematicians von Neumann (1951) and Ulam (1952), and “one can say that the ‘cellular’ comes from Ulam and the ‘automata’ comes from von Neumann” [47–49]. The final breakthrough of CA came with

John Conway's 'The Game of Life' in 1970. Urban CA is often defined by (1) a raster lattice representing the spatial context, (2) a set of states associating a cell with a certain land-use type, (3) neighborhoods influencing the spatial configuration and (4) transition rules regulating the conversion of a cell state with every (5) time step [12]. The gridded two-dimensional character of a CA environment makes it well suited for the simulation of urban land-use and land-cover conversion. Here, the most popular CA modeling urban growth was developed by the authors mentioned in references [48–55]. The progress of CA implementations profited heavily by innovations in remote sensing techniques. The world's radiances are recorded from a bird's eye view and stored regularly pixel-by-pixel. Hence, the world's surface is represented in a two-dimensional raster lattice facilitating a paradigm of modeling from the pixel. Natural or administrative borders are completely neglected so that land-use and land-cover patterns become the only things that matter. While maps always depend on a more or less subjective semiotics and imply reduced content, remotely sensed images provide the unmediated biophysical context of coupled human–environment systems [56]: By classifying a data set of radiances with the help of specific spectral characteristics, a continuous spatial texture is turned into a discrete spatial pattern. Accordingly, a classified time series of LANDSAT data of 1975, 1984, 2001 and 2005 is applied for his study. The data sets were classified using a hybrid approach of supervised classification algorithms and knowledge-based decision trees. The resultant classification simply identifies 'urban' and 'nonurban' areas, where an "urban" area is defined as having a surface imperviousness of a minimum of 25%. A validation analysis of the classification documented an accuracy of >85%. In order to balance the spatial resolution and the spatial extent of the Ruhr, a grid resolution of 100 m was used. This classification procedure is described in detail in references [21, 61]. For the calibration of SLEUTH, the 1984 data comprise the base year and the 2001 data constitute the reference year. For the validation of SLEUTH, the 1975 data serve as the base year and the 2005 data constitute the reference year. Finally, the urban growth detected in the classified LANDSAT data between 1984 and 2001 is used to train the SVM model.

3. Modelling urban growth with an optimized cellular automaton

3.1. SLEUTH – An urban cellular automaton

Clarke's urban growth model (UGM), mostly identified as SLEUTH, understands urbanization as a diffusion process where complex urban patterns spread as a whole. It has been applied in several urban growth studies all over the world [19] and offers many set screws for an enhancement of its performance. SLEUTH is an acronym of its initial input factors, which are slope, land-use, exclusion, transport and hillshade. The base data consist of the urban land-use configuration and the mandatory slope and transportation layer. The exclusion layer is optional, but recommended because it prevents the location of urban cells in, for example, conservation areas or water bodies. Additionally, the exclusion layer can be combined with a probability map to enhance the simulation performance. Five growth coefficients (dispersion, breed, spread, slope and road gravity) define the four growth rules of SLEUTH: spontaneous growth, representing the random emergence of new urban areas;

new spreading center growth; edge growth depicting extensive urban sprawl and road-influenced growth (**Figure 2**). The last one is SLEUTH-specific and relocates a temporary cell along the road to its final position. Space and time are treated discretely in the CA. Thus, one growth cycle represents 1 year of urban growth and consists of the four aforementioned successive growth simulations. Each selected new urban cell is tested against the local slope and exclusion information as well as a random value during each growth cycle. One model step consists of all growth cycles (years) between the starting and the end date of the calibration phase.

Figure 2. Growth types of a growth cycle in SLEUTH.

The calibration process of SLEUTH is based on the brute-force method. Every parameter combination of the particular growth coefficients between values of 0 and 100 is tested until the optimal balance is assessed. Every modeling process for each parameter combination is run several times by using Monte-Carlo (MC) iterations. Goetzke modified SLEUTH and implemented it into XULU (eXtendable Unified Land-use Modeling Platform), a modeling environment developed at the University of Bonn [57, 58]. The standard calibration evaluation

method of SLEUTH has been replaced by the multiple resolution validation (MRV) [59]. The MRV procedure compares an observed simulated map with a validation map at different spatial resolutions. High -resolution maps are weighted more than maps at lower resolution. The basic idea behind MRV is to attenuate the impact of localization errors by extending the conventional cell-by-cell comparison and considering the similarity of the entire neighborhood of a cell. Thus, the ‘fuzziness’ of categorical maps is addressed [58], and spatial patterns can be simulated quite precisely by accurately classifying only a relatively few map cells. Additionally, urban land-use calibration with MRV requires only two maps: a map of the initial calibration year and one of the final year.

3.2. Support Vector Machines

In their contemporary form, SVM was firstly formulated by Cortes and Vapnik [20]. Along with artificial neural networks and genetic programming they represent a new generation of machine learning algorithms. With their robust operation architecture and their valid classification results, SVM is a very popular classification technique for remote sensing data [60]. Fundamentally, SVM is a linear binary classifier that labels a sample of empirical data by constructing the optimal separating hyperplane (**Figure 3**, left). Traditional machine learning methods try to minimize the empirical training error, causing a tendency to overfit [61, 62]. They are strongly tailored to the training data, so extending them to additional data becomes difficult. According to the principles of structural risk minimization, SVM tries to minimize the upper bound of the expected generalization error through maximizing the margin between the separating hyperplane and the data. The margin concept is the key element in the SVM approach for it is an indicator of its generalization capability [63, 64].

Figure 3. An optimal hyperplane constructed by the support vectors separates the training data (left). To solve a non-linear classification problem, the input data is projected onto a higher-dimensional Hilbert space (right) [65].

The principal advantage of SVM is the option to transform the model in order to solve a nonlinear classification problem without any a priori knowledge. Using the so-called ‘kernel trick’ (Eqs 7–9), the input vectors are reprojected to a higher dimensional space in which they can be classified linearly (**Figure 3**, right).

Considering the scenario of a set of training vectors T belonging to two classes:

$$T = \{(x_i, y_i) : i = 1, \dots, n\} x_i \in \mathbb{R}^n, y_i \in \{-1, 1\} \quad (1)$$

where

y_i = the class label (here urban growth and no urban growth)

x_i = a given data point in the n -dimensional feature space.

In this scenario, the dimension of the input space is determined by the range of urban growth driving forces. A hyperplane needs to be found which separates the positive from the negative feature vectors. The ‘separating hyperplane’ H can be parameterized linearly by w and b

$$H : \langle w, x \rangle + b = 0 \quad (2)$$

where w , element of $\mathbb{R}^d$, is a normal to H and b , element of $\mathbb{R}$, the bias. The classification problem can be formalized as the decision function

$$\text{sgn}(f_{(x)}) = \text{sgn}(\langle w, x \rangle + b) \quad (3)$$

For the linearly separable case, two hyperplanes H_+ and H_- are constructed by the closest positive and negative, respectively, examples – the so-called support vectors:

$$H_+ : \langle w, x \rangle + b = 1 \text{ and } H_- : \langle w, x \rangle + b = -1 \quad (4)$$

Note that H_+ and H_- are parallel because they have the same normal and no training points fall between them. Through the perpendicular distances from the origin of H_+ and H_- it can be shown that the distance between the optimal separating hyperplanes H_+ and H_- , respectively, H_+ and H , is $1/\|w\|$ where $\|w\|$ is the Euclidean norm of w . So the margin between H_+ and H_- is $2/\|w\|$. The optimal separating hyperplane can be found where the margin between H_+ and H_- is the largest. Hence $\|w\|$ has to be minimized. The formulation of the constrained optimization problem is

$$\begin{aligned} \min_{w, b} \quad & \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i \\ \text{subject to } & y_i (\langle w, x_i \rangle + b) - 1 \geq 0 \text{ for } i = 1, \dots, n \end{aligned} \quad (5)$$

The constant C is called penalty parameter and ξ_i is a slack variable representing the error in the classification. The first part of the objective function tries to maximize the margin between the two classes and the second part minimizes the classification error. The optimization problem is solved by formulating it in a dual form derived by constructing a Lagrange function according to the Karush-Kuhn-Tucker optimality condition [63]. The resulting classification rule is

$$\text{sgn}(f_{(x)}) = \text{sgn} \sum_{i=1}^n \alpha_i y_i (\langle x_i, x \rangle + b) \quad (6)$$

where α_i values are the corresponding Lagrange multipliers to x_i and b is the constant. The support vectors are all x_i where $\alpha_i \neq 0$. If the classification problem is not separable linearly, then the decision function cannot be solved simply with the separation approach described above. The data set must be transferred or projected respectively into a higher dimension: the Hilbert space. This process extends the methods of vector algebra from two-or three-dimensional spaces to spaces depicting any finite or infinite number of dimensions (**Figure 3**). By using the function ϕ with $d1 < d2$, the number of possible linear separations is increased:

$$\mathbb{R}^{d1} \rightarrow \mathbb{R}^{d2}, x \rightarrow \phi(x) \quad (7)$$

SVMs are well suited for this operation since the training data x_i emerge only in scalar products in terms of the optimization problem. The scalar product x_i, x is calculated in the higher dimensional space $\phi(x_i), \phi(x)$. The transfer is performed with the use of a kernel function k according to Mercer's theorem [65].

$$k_{(x_i, x)} = \langle \phi_{(x_i)}, \phi_{(x)} \rangle \quad (8)$$

The Gaussian radial basis kernel function is a reasonable first choice ([64, 71]):

$$k_{(x_i, x)} = e^{-\gamma |x - x_i|^2} \quad (9)$$

The parameter γ defines the width of the Gaussian kernel function. After the kernel trick the decision function becomes

$$\text{sgn} f_{(x)} = \text{sgn} \sum_{i=1}^n \alpha_i y_i k(x_i, x + b) \quad (10)$$

Instead of predicting the label directly, the class probability is calculated (Eq 11) which delivers the basis for the probability maps of urban growth. Platt approximates the probabilities for binary SVMs using a sigmoid function

$$P(y=1 \mid x) = \frac{1}{1 + e^{A + f_{(x)} B}} \quad (11)$$

where A and B are parameters estimated by minimizing the negative log-likelihood function [67].

3.3. Optimizing SLEUTH

In this study, SVM is applied to raster layer stack consisting of different geophysical, socioeconomic as well as demographic driving factors of urban growth in order to optimize the CA SLEUTH. The selection is based on recent empirical studies dealing with urban sprawl in Central Europe [2, 5, 24]. Most studies of SVM in the context of urban growth modeling employ ordinary distance variables to represent proximity [66, 68]. In some cases, varying accessibility has a significant effect on the forces driving land use decisions. Hence, the effects of accessibility to markets or important infrastructure facilities are measured by weighting distances with a road variable that was derived using a categorized road network data set. Demographic and socioeconomic data that are exclusively available at the district level have been disaggregated to dasymetric maps [69]. For the other socioeconomic variables that are not related to population, statistical data were projected to the center points of each district and inverse distance weighting was used for interpolation. To minimize spatial autocorrelation effects, a stratified sampling method was applied [70]. This procedure generated a training data set containing 4000 image pixels for each urban growth and no urban growth class, with a 1 km minimum separation distance between equal pixels. For the construction of the SVM model one can use the software tool imageSVM® implemented in the EnMAP Toolbox®. Originally, imageSVM was created for solving classification problems in the context of multi- and hyperspectral satellite imagery [71]. The output of a SVM classification with imageSVM is not only a classified binary image but also a probability image based on the principles of (Eq 11). The crucial step for constructing a SVM model is determining optimal parameter settings, including appropriate values for the penalty parameter C (Eq 5) and the kernel parameter γ defining the width of the RBF kernel (Eq 9). An effective method for balancing the accuracy results of ‘known’ training data with ‘unknown’ testing data is the n -fold cross validation procedure [70]. According to the ‘curse of dimensionality’ and the Hughes’ phenomenon, which describes the degradation of the classifier performance when increasing the number of features, it is additionally advisable to select the optimal feature combination [71, 72]. A common element of SVM feature selection is a forward feature selection, which initially trains each feature of the input feature set. The best performing feature is selected and the remaining features are used for training in combination with the initially selected one. The procedure is repeated until all features have been selected.

The driving forces (**Table 1**) form the feature space (Eq 2) and build the base for training the 1984–2001 SVM urban growth model. The rank of a variable within the SVM feature selection (**Table 1**) is a reliable indicator for assessing the influence of the urban growth driving forces that were selected as model input parameters [70]. Following several subsequent feature selections, nine variables were eliminated. It can be stated that the characteristic attributes of the distance-related variables [73] and of the number of jobs are more suitable for constructing the SVM model than other socioeconomic or demographic variables. The distance to the next railway station in particular seems to be a very good indicator for a possible urbanization. This

might be a link to the industrial past traversing the urban area by a freight transport network. Beside elevation – and slope, which already is a part of SLEUTH – no other geophysical variable is usable for the selection of areas suitable for urban growth with SVM. The parameters “Jobs” related to the labor market and “NetDwellArea” variable which is a descriptor of living conditions are other important urban growth drivers.

Name	Description	Rank*
Distance-related variables		
Dist Airport	Cost-weighted distance (CWD) to next international airport	5
Dist City	CWD to next city >25.000 inhabitants	3
DistHighway	CWD to next highway exit	2
Dist Railway	CWD to next railway station	1
Dist River	Euclidian distance to next river	6
Highway Buffer	500 m buffer to highways	n.i. ^x
Geophysical variables		
Elevation	Elevation above sea level (m)	11
Soil depth ^o	Vertical extent of soil layer (cm)	n.i.
Soil type ^o	Soil type defined by grain size (nominal)	n.i.
Soil quality ^o	Agricultural appropriateness (from [temporary] ‘not usable’ to ‘very good agricultural location’)	n.i.
Waterlogging ^o	Waterlogging type (from ‘low’ to ‘very high’)	n.i.
Water table	Depth of complete water saturation below ground (cm)	n.i.
Socioeconomic variables		
Income	Inverse distance-weighted (IDW) average income per month in district 1991	n.i.
Jobs	IDW number of jobs 1991	4
Land Price	IDW land value 1990	7
NetDwellArea	IDW per capita net dwelling area 1990	8
Unemployment	IDW unemployed per population 1991	9
Demographic variables		
Cars	Number of cars in district; density function (10 km kernel) DF	n.i.
Migration25–50	Difference between in- and out-migration per settlement of the group aged 25 to 50	n.i.
PopDens	Population density 1984; DF	10
[*] Rank according to the forward feature selection. ^x Not included. ^o Dummy coded.		

Table 1. Variables selected for SVM model.

Figure 4. SVM probability map of urban growth from 1984 to 2001.

The output of the imageSVM® classification is not only a classified land-cover image but also an image containing the probabilities of each pixel for ‘urban growth’ and ‘nonurban growth’ [66]. The receiving operator characteristic (ROC) is an approved index for the accuracy assessment of binary categorical probability estimations [74]. The ROC divides the probability outcomes into percentile groups from high to low probability and compares the individual probability groups with the cumulative real values. The ROC only considers the positive values estimated by the model; in our case all urban growth cells. To define the ROC, true positive and false positive rates are plotted for every percentile group. The result is a curve where the area under the curve (AUC) is the measure that represents the ROC statistic. If a model acts randomly, then the curve will be a line through the origin with a slope of 1 and an AUC of 0.5. If a model acts perfectly, then the AUC is 1. **Figure 4** shows the ROC of the SVM model as well as the created probability map and the observed urban growth between 1984 and 2001. The curve of the SVM model clearly reaches a stable level already at low percentile groups. The resulting AUC values confirm the visual impression. The SVM model achieves a value of 0.94 – an outstanding performance for the AUC.

3.4. Calibration and validation of SLEUTH-SVM

Together with the SVM-based allocation probability map of urban growth, SLEUTH-SVM is calibrated using the produced urban land-cover maps 1984 and 2001 as the start and the testing year. For the validation of the model, the predicted urban growth is compared with the

observed urban growth of 2005, starting the simulation in 1975. It is clearly distinguished between the data sets used for calibration, and the data set used for validation of the model. The SVM probability map based on various driving forces of urban growth is combined with the exclusion layer of SLEUTH. In total, the three different versions of SLEUTH are compiled:

- SLEUTH: without exclusion layer.
- SLEUTH-AR: exclusion layer (areas where urban growth is restricted such as water bodies, natural reserves, etc.).
- SLEUTH-SVM: exclusion layer and probabilities for urban growth based on the SVM analysis.

Figure 5. Agreement results of SLEUTH-SVM: comparison map of observed and predicted urban areas 2005.

The validation of complex system models such as CA not only includes careful error estimation but also addresses the uncertainty of the model results [75]. Unwin defines uncertainty in the context of spatial simulations as a measure of doubt and distrust in results which can be seen as a certain kind of vagueness due to stochastic variability [76]. Aerts et al. [77] demonstrated that a detailed examination of the outcomes after 100 MC iterations is a valid procedure for assessing the uncertainty of CA like SLEUTH. The resulting map shows how often a certain cell has been depicted by the model to be urbanized. In order to transform it into a binary land-use map, a probability of 33% as cut-off value is used which was elaborated via a standard

histogram frequency method [78, 79]. With this value the best balance between location and quantification performance could be achieved.

Figure 5 contains the comparison map of the predicted and the observed urban growth for 2005. It is important to emphasize that SLEUTH is a purely growth-oriented model. The CA exclusively models the transformation from nonurban to urban cell states. There is no ability to model in a spatially explicit manner the reverse process of urban contraction due to demolition or removal of sealed surfaces. In the near future, however, regional planning will have to deal with this process of extensive urban demolition (or urban perforation). For the 1975–2005 study period, spatial urban growth occurred concurrently with a contracting population [34]. There are only few areas where the simulation acts ‘false-positively’, meaning the model predicted urban growth where no growth has occurred [76]. These are nearly always located in open-spaced inner city areas or clustered along recreational parks of the river Emscher between Bottrop and Essen. In contrast, there are more areas where the model simulates ‘false-negatively’, which is predicting persistence where urban areas have spread in reality. Admittedly, it is virtually impossible to allocate greenfield development with industrial estates or the emergence of new traffic areas with a spatial certainty of 100 m without any local planning knowledge. Indeed, the urban areas in the district of Ennepe-Ruhr should have been actually captured. It seems that the slope layer of SLEUTH suppressed urbanization in this hilly region during the simulation run. However, in total, 108,220 ha of built-up land were predicted in the Ruhr for 2005. This is a growth of nearly 14% since 1975. In comparison, the observed urban growth rate is 39%. The underestimation of the quantity of change is specific for spatially explicit land-use change models [59, 80, 81]. For this reason, the model is validated regarding its overall simulation performance (overall agreement) in comparison with randomness (Cohen’s Kappa), the quantity estimations of urban growth (κ_{histo}), the allocation ability of urban growth (κ_{loc}), as well as the fuzziness of urban growth (F_i) (**Table 2**).

	SLEUTH	SLEUTH-AR	SLEUTH-SVM
New urban cells (ha)	110,668	108,220	110,445
Overall Agreement	0.911	0.912	0.914
Kappa	0.777	0.779	0.782
F_i^*	0.923	0.924	0.926
κ_{loc}	0.884	0.887	0.911
κ_{histo}	0.879	0.878	0.859

* F_i is the mean factor of agreement over all resolutions of the MRV.

Table 2. Validation results 1975–2005 of SLEUTH.

The achieved results are on a very good level. They show that the optimized CA SLEUTH-SVM outperforms the SLEUTH model without any exclusion information as well as the SLEUTH model exclusively containing the restriction areas. The lower quantification per-

formance is due to the simulation algorithm of SLEUTH: if SLEUTH is run without a probability map or an exclusion layer, then nearly every cell has the same probability of urbanization. Utilizing probability maps increase the possibility that a particular cell is defined as not suitable for urbanization and the resulting growth rate decreases. In several urban land-use change studies, a low signal of urban growth in comparison to a very high signal of persistent nonurban cells was discussed [59, 81]. κ_{loc} is a suitable measurement to assess the allocation accuracy of a land-use model. Additionally, the model’s ability of allocating newly urbanized cells should be tested. The null model comparison is a rational choice. A null model is a map containing the initial land-use pattern; it can therefore also be thought of as a pure persistence-map. Thus, null models regularly achieve better results at high resolutions than the actual land-use model; no change predicted means there are no allocation errors of urbanized areas. At a certain spatial resolution, the quantity error of a null model increases so that the predicted map achieves better results. The resolution level where the agreement factor of the land-use model outperforms the null model for the first time is called ‘null resolution’.

Figure 6. MRV curves of the applied models.

The MRV results show a consistently excellent level of overall accuracy. This can be attributed to the ability of all three models to almost perfectly predict the location and the quantity of nonurban growth cell states. SLEUTH-SVM is the only model exceeding the level of the null model already at the resolution level 1 of 100 m (Figure 6). The agreement curve of the null model forms a straight line, reflecting the low signal of urban growth in comparison to the very high signal of persistent nonurban growth cells. Again, the optimized version of SLEUTH

shows a higher agreement between the predicted and the observed urban growth on the level of high resolutions up to 400 m than SLEUTH and SLEUTH-AR. As soon the resolution gets coarser, the impact of allocation errors decreases and the performance of SLEUTH-SVM stagnates.

The question of how the SVM-probability map influences the spatial extension of the Ruhr's urban growth will be analyzed with the concept of urban DNA [82]. Analogous to the biological DNA, it postulates fundamental elements that are common to each urban area and determine their future growth pattern [83]. Gazulis and Clarke apply the concept to an abstract space representation mimicking the variable input of SLEUTH [84]. Hence, this grid image reflects a kind of digital petri dish consisting of an urban area, a slope layer, transport information as well as exclusion areas (**Figure 7**). The urban input is just a single urban cell in the middle of the image whereas all other cells are defined as nonurban. The slope has a minimum value of 0% and increases concentric-radially to a maximum value which is equal to the maximum slope value to be found in the Ruhr (70%). The transport network is represented by a single road crossing the center of the image from north to south. In this study, the exclusion layer is exchanged by the SVM probability map of urban growth of the Ruhr. For estimating the spatial impact of the SVM optimization procedure, the particular probability map is allocated with a linear transition from high to low probabilities equivalent to their particular value range. In the south of the urban center, the probabilities decrease from 1 to the particular medium value. This medium level continues northwards from the urban center and decreases to zero. Thus, the maps are divided lengthwise from west to east.

Figure 7. Urban simulation in a digital petri dish consisting of the fundamental elements of the Ruhr's urban area.

The models SLEUTH and SLEUTH-SVM are run with the calibrated growth coefficients and 100 MC iterations. Hence, one can observe the allocation behavior of the CA under the SVM-defined conditions of the Ruhr's urban areas. The border of high and medium probabilities of urban growth is distinct in the SVM-optimized version of SLEUTH. The CA is clearly guided

whereas the regular version allocates the cells more randomly in the surroundings of already built-up areas. In the northern part of the synthetic region, the urban pattern is slim while in the southern part it broadens. All in all, the DNA of the Ruhr's urban areas reveals a tendency to edge growth and a high influence of the road network. The SVM-based probability optimizes the allocation performance of the urban CA SLEUTH.

4. Conclusion and outlook

The aim of this study was to optimize the CA SLEUTH by using SVM and to assess its performance in comparison to its standard configuration. A SVM-based probability map including the impact of driving forces on the allocation of new urban areas was combined with the exclusion layer of SLEUTH. Hence, the model could be guided and its stochastic variability regarding the emergence of urban cells depressed. The application of SVM additionally delivered insights into the most important factors driving the local urbanization suitability. Thus, the CA provided a theoretical foundation. The importance of distance-related variables over socioeconomic or demographic variables in the SVM model was clear. Geophysical variables were not useful to select areas suitable for urban growth with SVM. The models have been applied to the polycentric agglomeration of the Ruhr. The region's specific settlement structure is characterized by large urban areas solely divided through administrative borders. The scattered rural districts complete the image of a challenging study region in terms of organizational hierarchies, migration flows and heterogenic growth conditions. The accuracy of SLEUTH-SVM has been assessed regarding the overall agreement, the fuzziness, the ability to allocate new urban cells, the performance in comparison with the randomness as well as the quantity and the allocation ability of urban growth. The calibration and the validation of the model have been separated carefully. The validation indices for SLEUTH-SVM showed good values around 0.91 (kappa) and 0.93 (MRV). As a reliable result, it can be stated that the allocation performance of SLEUTH is optimized clearly when coupling it with a SVM-based probability map. Its spatial impacts are visualized with the concept of urban DNA and a digital petri dish. Hence, the generic growth elements of the Ruhr's urban area were uncovered.

As a next step, coupling different modeling techniques for prediction and process analyses of urban land-use and land-cover change should be pushed beyond the physical restriction of pixels. To incorporate the irrational human component impacting on all spatial and temporal levels between the household and the global scale, pixels must be coupled with people. This can, for instance, be done by extending the enhanced version of SLEUTH with a multiagent system. That way, one can study emergence phenomena resulting from complex behavioral interaction processes on the micro scale. Hence, the simulation of urban change could be extended from analyzing growth processes to the estimation of urban decline. Coupling actors with factors would be a chance to overcome formal, differential equations. Therefore, the present ride on the surface of an ocean of driving forces, pressures, states, impacts and responses would be optimized into diving right into it.

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