Intensity Analysis and the Figure of Merit's Components for 1 assessment of a Cellular Automata - Markov simulation model 2 Orsolya Gyöngyi Varga¹, Robert Gilmore Pontius Jr², Sudhir Kumar Singh³, Szilárd Szabó⁴ 3 4 5 ¹ Department of Physical Geography and Geoinformatics, Faculty of Science and Technology, 6 University of Debrecen, Debrecen, Hungary 7 ORCID: 0000-0002-2060-945X 8 9 ² School of Geography, Clark University, Worcester, MA 01610, USA ORCID: 0000-0001-7287-5875 10 11 ³ K. Banerjee Centre of Atmospheric & Ocean Studies, IIDS, Nehru Science Centre, University 12 13 of Allahabad, Allahabad, Uttar Pradesh, India 14 ORCID: 0000-0001-8465-0649 15 ⁴ Department of Physical Geography and Geoinformatics, Faculty of Science and Technology, 16 17 University of Debrecen, Debrecen, Hungary ORCID: 0000-0002-2670-7384 18 19 20 Corresponding author: 21 Orsolya Gyöngyi Varga, e-mail address: varga.orsolya.gyongyi@gmail.com 22 23 Abstract 24 Some popular metrics to evaluate land change simulation models are misleading. Therefore, 25 land change scientists have called for the development of methods to evaluate various aspects 26 of modelling applications. This article answers the call by giving novel methods to compare 27 three types of land change: 1) reference change during the calibration time interval, 2) 28 simulation change during the validation time interval, and 3) reference change during the 29 validation time interval. We compare these changes by using Intensity Analysis' three levels 30 and the Figure of Merit's four components: Misses, Hits, Wrong Hits and False Alarms. We illustrate the concepts by applying a Cellular Automata - Markov land change model to a case 31 32 study in northeast Hungary. We used reference maps of five land categories to calibrate the 33 model during 2000-2006, then to validate the simulation during 2006-2012. Intensity Analysis' 34 time interval level shows that the simulation change and the reference change decelerated from 35 2000-2006 to 2006-2012. Intensity Analysis' category level shows that the simulation losses 36 were less than what a pure Markov chain would have dictated. Intensity Analysis' transition 37 level shows that the model's Markov algorithm simulated correctly that the gain of Forest 38 targeted Agriculture and Wetland. The Figure of Merit's components reveals more allocation 39 error than quantity error. Our collection of metrics show that more error derived from the 40 Cellular Automata algorithm than from the Markov algorithm. We recommend that scientists 41 use Intensity Analysis and the Figure of Merit's components to reveal various fundamental 42 aspects of modelling applications. 43

44 Keywords

45 cellular automata, CA-Markov, Figure of Merit, Intensity Analysis, land change, validation.

- 47 **Conflicts of Interest**
- 48 The authors have no conflicts of interest.
- 49

50 Acknowledgements

51 The United States National Science Foundation (NSF) supported this work via the Long 52 Term Ecological Research network via grant OCE-1637630 for Plum Island Ecosystems. On 53 behalf of Dr. Szilárd Szabó, our article was supported by the EFOP-3.6.1-16-2016-00022 and 54 the TNN 123457 projects. The projects were co-financed by the European Union and the 55 European Social Fund. Anonymous reviewers supplied constructive feedback that helped to

improve this article.

58 Highlights

- 59 1. Scientists should use better methods to assess models that simulate change.
- 60 2. We give novel metrics to reveal differences among three time intervals.
- 61 3. Intensity Analysis reveals various types of quantity disagreements through time.
- 62 4. FOM's components distinguish quantity from allocation disagreement during validation.
- 63 5. The CA part caused more error than the Markov part in a CA-Markov simulation.

65 **1 Introduction**

Land change models can simulate future changes among land categories (Camacho 66 67 Olmedo et al. 2018). Use of such models can give insight concerning management options. For example, extrapolation of recent trends can help to anticipate threats to habitats (Bierwagen et 68 69 al. 2010; Hepinstall et al. 2008; Szabó et al. 2012; Ziółkowska et al. 2014). Proper insight 70 requires that modellers understand how model behavior compares to landscape behavior, which 71 presents several challenges. Therefore, scientists have called for more research into land-change 72 modelling (Paegelow et al. 2013; Pontius Jr et al. 2018; National Research Council 2014). 73 Specifically, Brown et al. (2013) urge that "more needs to be done to develop and disseminate 74 methods for evaluating land-change models". Our article responds to these challenges by 75 presenting methods to compare simulated change to reference change by applying a collection 76 of metrics that give deeper insights than existing popular metrics.

Empirical models typically examine historic patterns of land change during a calibration time interval, and then extrapolate those patterns beyond the calibration time interval. Models simulate temporal change during the extrapolation in terms of two concepts: quantity and allocation. The quantity concerns the size of each transition from one category to another. The allocation concerns the spatial distribution of each transition. Models' algorithms frequently specify the quantity separately from the allocation.

Markov models can describe each transition's quantity. A Markov matrix specifies the
proportion of each category that transitions to another category during each time interval. The
empirical Markov matrix during the calibration time interval can extrapolate the quantity of
each transition beyond the calibration time interval by applying a Markov chain (Baker 1989).
A Markov chain is a popular method of extrapolation in land change models.

88 Cellular Automata (CA) can guide each transition's allocation. CA models consist of a 89 regular grid of cells and rules that dictate how each cell's neighbours influence the future 90 category of each cell (Sipper 1997). CA models typically simulate transitions in cells that are 91 near the borders between categories. Neumann and Ulam introduced cellular automata in the 92 1940's to see whether mathematical formulas and logical rules can describe self-reproduction 93 of biological systems (Benenson and Torrens 2004).

CA-Markov models combine a Markov algorithm to simulate the quantity of change
and a CA algorithm to simulate the allocation of change (Singh et al. 2015). Researchers have
applied CA-Markov models to various case studies (Jalerajabi and Ahmadian 2013; Paegelow
et al. 2014; Sang et al. 2011). Some studies compared CA-Markov with other land change
models, such as GEOMOD and Idrisi's Land Change Modeller (Camacho Olmedo et al. 2015;
Pontius and Malanson 2005).

100 CA-Markov is one type of model that simulates transitions among categories, while 101 many others exist. For instance, SLEUTH is a CA model but SLEUTH does not use a Markov 102 matrix to extrapolate the quantity of each transition (Clarke et al. 1997; Silva and Clarke, 2001). 103 SLEUTH has been used for setting up scenarios under various conditions for forecasting urban 104 growth based on historical and contemporary conditions (Herold et al. 2003). Some models are 105 neither CA nor Markov. For example, some models focus on economic factors, where land 106 occupation is based on market conditions, such as in Computable General Equilibrium and Partial Equilibrium models (DeRosa et al. 2016). The structure of land change models vary 107 108 based on their purposes. Some researchers aim to analyse hotspots of land change at a national 109 level (Verburg et al. 2002) or at spatial resolutions as detailed as the household level (Evans 110 and Kelley, 2004). Some models project changes by analyzing socio-economic and environmental drivers together (Veldkamp and Verburg, 2004). There is a need to integrate 111 112 model results into landscape planning because environmental management is a typical purpose 113 (Lippe et al. 2017; Convertino and Valverde Jr., 2013). It is useful to know the implications of 114 an extrapolation of recent trends so that decision-makers can understand the trajectory of the system. Regardless of model selection or purpose, modellers should know three aspects of any application: 1 how the model characterizes change during the calibration interval, 2 how the model extrapolates the change during a validation interval, and 3 how the extrapolated change compares to the reference change during the validation interval.

119 Some scientists compared the model's output map at the final time point of the 120 validation interval to the reference map at the same time point to measure the accuracy of the 121 simulation (Yang et al. 2014; Halmy et al. 2015; Singh et al. 2015, Mishra and Rai 2016; Keshtkar and Voigt 2016; Chakraborti et al. 2018). That comparison cannot give insight to 122 123 temporal change, because both maps show the same time point. Therefore, that two-map 124 comparison cannot distinguish between correctly simulated change and correctly simulated 125 persistence during the validation time interval. If persistence dominates a landscape, then the 126 two-map comparison typically gives large values for percent correct and kappa, regardless of 127 whether the model simulates change correctly. In order to avoid this conceptual blunder, 128 Pontius Jr et al. (2008, 2011, 2018) recommend the use of three maps to compare simulation 129 change versus reference change during the validation time interval. The three maps are: 130 reference at the start of validation interval, simulation at the end of validation interval, and 131 reference at the end of validation interval. The Figure of Merit (FOM) is a popular metric for 132 model validation using this three-map comparison (Klug et al. 1992; Perica and Foufoula-Georgiou 1996). The FOM ranges from zero to one, where zero means no intersection between 133 134 simulation and reference change while one means perfect intersection between simulation and reference change. The FOM has limited ability to offer insight because the FOM is a single 135 136 metric that combines information concerning quantity and allocation. For example, the FOM 137 fails to reveal how the quantity of simulated change compares to the quantity of reference change. Furthermore, FOM fails to show how quantity disagreement compares to allocation 138 139 disagreement. Our article shows how to compute and interpret FOM's components in a manner 140 that distinguishes between quantity and allocation.

141 Intensity Analysis can offer insights to modelling applications because Intensity 142 Analysis is a framework to reveal various patterns of change among categories across time 143 intervals (Aldwaik and Pontius Jr 2012; Aldwaik and Pontius Jr 2013). Intensity Analysis has 144 three levels, where each increasing level examines increasingly detailed information given the 145 previous level. Intensity Analysis has become popular to analyse temporal changes among 146 categories (Castro and Rocha 2015; Raphael John et al. 2014; Yang et al. 2017; Quan et al. 147 2018; Rocha et al. 2017; Aabeyir et al. 2017; Zhou et al. 2014; Huang et al. 2018; Huang et al. 148 2012). To the best of our knowledge, our article is the first to use Intensity Analysis to evaluate 149 the application of a simulation model.

150 There are various reasons why the simulation change might not match the reference 151 change during the validation interval. First, the reference change might not be stationary from 152 the calibration interval to the validation interval, in which case empirical calibration would 153 likely produce an extrapolation that lacks predictive power. Second, the model might simulate 154 processes that do not exist in the landscape, such as Markov processes that dictate the quantity 155 of change or neighbourhood processes that dictate the allocation of change. Therefore, proper 156 interpretation requires clear methods to compare three time intervals: 1) reference change 157 during the calibration interval, 2) simulation change during the validation interval, and 3) 158 reference change during the validation interval. Previous methods focused exclusively on the 159 validation interval, which offers helpful but limited insight because such methods fail to consider differences between the calibration and validation intervals. One of the innovations of 160 161 our article is that we compare the calibration interval to the validation interval.

We illustrate the concepts using a case study in Northeast Hungary. We applied Idrisi
 Selva's CA-Markov model, and then evaluated the application by using Intensity Analysis and
 the FOM's components. We compare three time intervals: reference 2000-2006, simulation

2006-2012, and reference 2006-2012. Our objective is to show how Intensity Analysis and
FOM's components offer valuable insights concerning how model behavior relates to landscape
behavior. The combined use of these measurements and the comparison of the calibration
interval to the validation interval are the two main innovations of our paper.

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170 **2 Methods**

171 *2.1 Study Site*

The study site is a 25 x 25 km region located around Tokaj city and the tributary of Tisza and Bodrog rivers in Hungary (Dövényi 2010). The site is a diverse landscape of five topographically different microregions. A large part of the region has been a nature reserve since 1986, and since 2002 has belonged to the Tokaj Wine Region Historic Cultural Landscape, which is a UNESCO World Heritage site (Kerényi 2015). The site's protected status restricts large land changes.

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179 2.2 Data and Simulation

180 We used maps of the Corine Land Cover (CLC), produced by the European 181 Environment Agency and managed by the Copernicus Land Monitoring Service 182 (https://land.copernicus.eu/pan-european/corine-land-cover). CLC data are popular for landscape monitoring and analysis, including in Hungarian study areas (Csorba and Szabó 183 184 2009; Túri 2010). Büttner et al. (2004) report the data have a thematic accuracy of at least 85%. 185 The CLC programme established land cover layers via visual interpretation of satellite images 186 at a 1:100,000 scale, minimum mapping unit of 25 hectares and width of linear objects of 100 187 m.

188 CLC categories have three hierarchical levels (Feranec et al. 2016). The most detailed 189 third level has 44 categories, of which 18 appear in our study region. We used the first level, 190 which has five aggregated classes, which we name Artificial, Agriculture, Forest, Wetland, and 191 Water. Table 1 describes our five land cover classes and their equivalent class in CLC 192 nomenclature. CLC data has been distributed in the standard European Coordinate Reference 193 System defined by the European Terrestrial Reference System 1989 (ETRS89) datum and 194 Lambert Azimuthal Equal Area projection (EPSG: 3035). We obtained vector maps at 2000, 195 2006, and 2012, and then converted them into 25 m spatial resolution raster layers in the 196 software Idrisi Selva.

197

Category in model	Category in CLC	Description of category in our study area
Artificial	Artificial surfaces	All urban facilities (including industrial areas) and mining sites
Agriculture	Agricultural	Mainly agricultural areas with various cultures (arable land, vineyards, fruit plantations, pastures, etc.)
Forest	Forests and semi-natural	Mainly broad-leaved and mixed forests with transitional areas into scrub
Wetland	Wetlands	Inland wetlands
Water	Water bodies	All forms of water bodies, including natural and man-made water bodies or rivers.

198 **Table 1.** Categories in our land change model along with the equivalent CLC category

199 (standard level I) and the content of each category.

We used the change during 2000-2006 to calibrate the CA-Markov model. The model then simulated changes during 2006-2012, which is the validation time interval. The CA-Markov model has distinct algorithms to simulate the quantity versus the allocation of each transition.

The model's Markov algorithm guides the simulation's quantity. The algorithm computes a Markov matrix based on the changes during the calibration time interval, and then uses a Markov chain to extrapolate the size of each transition during subsequent time intervals. The Markov chain assumes a constant proportion of each initial category transitions to every other category during each time interval.

The model's CA algorithm guides the simulation's allocation. The algorithm allows the simulation of a spatial process whereby each category gains near the edges of the category's initial patches (Eastman 2012; Mas et al. 2014). A spatial filter and an iteration number influence how near to the edges the changes occur. We used a 5-by-5 spatial filter and an iteration number of six, which are the model's default parameters. Idrisi Selva's CA-Markov model does not have automated calibration for these two parameters.

Figure 1 shows the maps that serve as the basis of our analysis. At all three time points,

Artificial accounts 5%-6% of the spatial extent, Agriculture for 72%-74%, Forest for 14%-16%,

218 Wetland for 4% and Water for 3%.



219 220

Figure 1 Reference maps of categories at three time points and of change during two time intervals in northeast Hungary. Persistence means a category remains the same during a time 221 222 interval.

224 2.3 Intensity Analysis

225 Intensity Analysis is a framework to understand the sizes and intensities of temporal changes among categories (Aldwaik and Pontius Jr 2012, 2013; Pontius Jr et al. 2013). Intensity 226 227 Analysis has three levels: Interval, Category, and Transition. The Interval level examines the 228 overall change during each time interval. The Category level examines the loss and gain of each 229 category during each time interval. The Transition level examines how the gain of a category 230 transitions from other categories during each time interval. We applied Intensity Analysis using 231 free software from http://www.clarku.edu/~rpontius/. The inputs were a crosstabulation matrix 232 for each of three time intervals: 2000-2006 reference, 2006-2012 simulation, and 2006-2012 233 reference.

Table 2 gives the mathematical notation for the equations of Intensity Analysis based on Pontius Jr et al. (2013). All time intervals have the same duration of six years; therefore, we did not use the equations of Aldwaik and Pontius Jr (2012), which compute annual change during time intervals that have various durations.

238

239	Table 2	Mathematical	Notation	for	Intensity	Analysis.
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Symbol	Meaning
C_{tij}	number of cells that are category <i>i</i> at start and category <i>j</i> at end of time
	interval t
C_{tji}	number of cells that are category <i>j</i> at start and category <i>i</i> at end of time
	interval t
G_{tj}	intensity of gain of category <i>j</i> during time interval <i>t</i> relative to size of
	category <i>j</i> at end of time interval <i>t</i>
i	index for a category
j	index for a category
J	number of categories
L_{ti}	intensity of loss of category <i>i</i> during time interval <i>t</i> relative to size of
	category <i>i</i> at start of time interval <i>t</i>
R_{tij}	intensity of transition from category <i>i</i> to category <i>j</i> during time interval <i>t</i>
	relative to size of category <i>i</i> at start of time interval <i>t</i>
S_t	change percentage during time interval t
t	index for a time interval
W_{tj}	uniform intensity of transition from all non- <i>j</i> categories to category <i>j</i> during
•	time interval t relative to size of all non-j categories at start of time interval t

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241 For the interval level, equation 1 defines S_t , which is the change percentage during each interval t. The change percentage S_t is the uniform intensity during interval t for the category 242 243 level. Equations 2 and 3 give the category level intensities of loss L_{ti} and gain G_{ti} during interval 244 t. If change during interval t were distributed uniformly across the spatial extent, then $S_t = L_{ti} =$ 245 G_{ti} for all categories i and j. If $L_{ti} < S_t$, then the loss of category i is dormant during interval t. If $L_{ti} > S_t$, then the loss of category *i* is active during interval *t*. Similarly, if $G_{ti} < S_t$, then G_{ti} is 246 247 dormant; and if $G_{ti} > S_t$, then G_{ti} is active. If the status as dormant or active is the same during 248 sequential time intervals, then we say the category's loss or gain is stationary. The loss intensity L_{ti} is identical to the diagonal entry in a Markov matrix for interval t concerning category i. 249

250
$$S_t = \frac{(\text{size of change during interval } t)100\%}{\text{size of spatial extent}} = \frac{\left\{\sum_{i=1}^{J} \left[\left(\sum_{j=1}^{J} c_{tij}\right) - c_{tii} \right] \right\} 100\%}{\sum_{i=1}^{J} \left(\sum_{j=1}^{J} c_{tij}\right)}$$
(1)

251
$$L_{ti} = \frac{(\text{size of loss of } i \text{ during interval } t)100\%}{\text{size of } i \text{ at start of interval } t} = \frac{\left[\left(\sum_{j=1}^{J} C_{tij}\right) - C_{tii}\right]100\%}{\sum_{j=1}^{J} C_{tij}}$$
(2)

252
$$G_{tj} = \frac{(\text{size of gain of } j \text{ during interval } t)100\%}{\text{size of } j \text{ at end of interval } t} = \frac{\left[\left(\sum_{i=1}^{J} C_{tij}\right) - C_{tjj}\right]100\%}{\sum_{i=1}^{J} C_{tij}}$$
(3)

253 For the transition level, equation 4 gives the transition intensity R_{tii} from category i to category j during time interval t. Equation 5 gives the uniform intensity W_{ti} for the gain of 254 category *j* from categories that are not *j* at the interval's start time. The order of subscripts *j* 255 and i in C_{tji} in the denominator of equation 5 is intentional, so that the summation over i 256 257 subtracts category *j* at the interval's start time. If category *j* were to gain uniformly from all other categories, then $W_{tj} = R_{tij}$ for all *i*. If $R_{tij} < W_{tj}$, then the gain of *j* avoids *i*. If $R_{tij} > W_{tj}$, 258 259 then the gain of *j* targets *i*. If the status as avoiding or targeting is the same during sequential 260 time intervals, then we say the transition is stationary. The transition intensity R_{tij} is identical 261 to the off-diagonal entry in a Markov matrix for interval t concerning the transition from 262 category *i* to category *j*.

263
$$R_{tij} = \frac{(\text{size of transtion from } i \text{ to } j \text{ during interval } t)100\%}{\text{size of } i \text{ at start of interval } t} = \frac{(C_{tij})100\%}{\Sigma_{j=1}^{J}C_{tij}}$$
(4)

264
$$W_{tj} = \frac{(\text{size of gain of } j \text{ during interval } t)100\%}{\text{size of not } j \text{ at start of interval } t} = \frac{\left[\left(\sum_{i=1}^{J} C_{tij}\right) - C_{tjj}\right]100\%}{\sum_{i=1}^{J}\left[\left(\sum_{j=1}^{J} C_{tij}\right) - C_{tji}\right]}$$
(5)

265 2.4 Figure of Merit's Components

266 We compare the simulation change to the reference change during 2006-2012 to gain insight concerning model validation. We perform the comparison visually by overlaying three 267 maps: reference 2006, simulation 2012, and reference 2012. We also perform the comparison 268 269 quantitatively by computing the components of the FOM. The FOM is a ratio, where the 270 numerator is the intersection of simulated and reference change, while the denominator is the 271 union of simulated and reference change. We used the 'lulcc package' of the R 3.3.3 software 272 to compute the FOM's components (Moulds et al. 2015; R Core Team 2017). Equation 6 shows 273 how the FOM derives from its four components: Misses, Hits, Wrong Hits and False Alarms 274 (Pontius Jr et al. 2011).

275 Figure of Merit =
$$\frac{(Hits)\ 100\%}{Misses + Hits + Wrong\ Hits + False\ Alarms}$$
(6)

where Misses = area of error due to reference change simulated as persistence; Hits = area of 276 correct due to reference change simulated as change; Wrong Hits = area of error due to reference 277 change simulated as change to the wrong category; False Alarms = area of error due to reference 278 279 persistence simulated as change.

280 FOM's components allow computation of quantity disagreement, allocation 281 disagreement and total disagreement (Chen and Pontius Jr 2010; Liu et al. 2014). Equation 7 282 gives quantity disagreement, while equation 8 gives allocation disagreement. Equation 9 shows 283 that the total disagreement is the sum of the quantity disagreement, allocation disagreement and 284 Wrong Hits. Wrong Hits are disagreement in the detailed respect that Wrong Hits are places 285 where the simulation map does not match the reference map at the end time of the validation 286 interval. Wrong Hits are agreement in the broad respect that Wrong Hits are places where change occurs according to both the simulation and the reference maps during the validation 287 288 interval.

$$290 \quad Allocation \ disagreement = 2 \ MINIMUM(False \ Alarms, \ Misses)$$

Total disagreement = Quantity disagreement + Allocation disagreement + Wrong Hits (9) 291

3 Results

295 *3.1 Intensity Analysis*

Table 3 shows the number of cells of each transition during three time intervals. One million cells exist the spatial extent; therefore, each entry in Table 3 divided by ten thousand gives the percentage of the spatial extent. The lower right entry shows that overall reference change during 2000-2006 is 17,107 cells, implying 1.7% of the spatial extent. Overall simulation change during 2006-2012 is 1.5%, while overall reference change during 2006-2012 is 1.1%.

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Table 3 Number of cells that transition from each row's start time category to each column's

and time category. For each transition, the top number gives 2000-2006 reference; the middle

number gives 2006-2012 simulation; and the bottom number gives 2006-2012 reference.

306 Persistence is a transition from a category to itself. Loss is the row's sum minus persistence.

	End Time						
Start Time	Artificial	Agriculture	Forest	Wetland	Water	Loss	
Artificial	50,107	44	0	1	0	45	
	55,837	0	0	0	0	0	
	55,762	9	66	0	0	75	
Agriculture	5,730	728,057	7,092	270	5	13,097	
	5,618	719,515	6,564	0	0	12,182	
	141	722,944	8,256	355	1	8,753	
Forest	0	415	140,508	3	5	423	
	0	0	147,959	0	2	2	
	550	436	146,969	3	3	992	
Wetland	0	2,812	359	36,770	0	3,171	
	0	2,390	325	34,329	0	2,715	
	0	145	528	36,371	0	673	
Water	0	369	2	0	27,451	371	
	0	361	0	0	27,100	361	
	1	2	8	711	26,739	722	
Gain	5,730	3,640	7,453	274	10	17,107	
	5,618	2,751	6,889	0	2	15,260	
	692	592	8,858	1,069	4	11,215	

308

309 Figure 2 shows results from Intensity Analysis' interval and category levels. The 310 uniform lines in each graph indicate the interval level in terms of overall change as a percentage 311 of the spatial extent. The model simulated deceleration of overall change from 2000-2006 to 312 2006-2012, while the simulation deceleration was not as severe as the reference deceleration. 313 Figures 2a and 2b show that the dormant or active status of each loss and gain during 2000-2006 was the same as during the simulation. If the software were to have simulated the sizes of 314 315 the transitions by using a Markov matrix exclusively, then the 2006-2012 simulation loss 316 intensities would be equal to the 2000-2006 reference loss intensities. However, figures 2a and 317 2b show that the 2006-2012 simulation loss intensities are less than the 2000-2006 reference 318 loss intensities. Figures 2a and 2c show that the reference patterns are not stationary from the 319 calibration interval to the validation interval. Most noteworthy, Wetland lost and Artificial 320 gained substantially during the calibration interval but not during the validation interval. 321 Therefore, the categorical intensities during the simulation do not match the reference during 2006-2012. Table 3 shows that Agriculture had the largest size of loss, but figure 2 shows that 322

Agriculture did not have the largest intensity of loss during all time intervals. The loss intensity for Agriculture was less than for Wetland because of Agriculture's large size, which is in the denominator of the intensity. Wetland had the greatest loss intensity during the calibration interval and the simulation, which was due in part to Wetland's small size in the denominator of the intensity.



328 329

Figure 2 Category intensities during three time intervals: (a) 2000-2006 reference, (b) 2006-

330 2012 simulation, and (c) 2006-2012 reference.

Figure 3 shows results of the transition level Intensity Analysis for the two largest gains: 331 332 Artificial and Forest. Comparison of the 2000-2006 reference and the simulation show how the 333 CA-Markov model extrapolated the intensity of changes from the calibration interval to the 334 validation interval. If the software were to have simulated the sizes of the transitions by using a Markov matrix exclusively, then the 2006-2012 simulation transition intensities would be 335 336 identical to the 2000-2006 reference transition intensities. The gain of Artificial is not stationary 337 through time. The gain of Artificial targeted only Agriculture during the calibration interval and the simulation. However, the reference gain of Artificial targeted only Forest during the 338 339 validation interval. In contrast, the gain of Forest is stationary across the three intervals with 340 respect to how the gain of Forest avoided or targeted the non-Forest categories.



Figure 3 Transition intensities for the gains of Artificial and Forest during three time intervals: (a-b) 2000-2006 reference, (c-d) 2006-2012 simulation, and (e-f) 2006-2012

- 344 reference.
- 345
- 346

347 3.2 Figure of Merit's Components

348 Figure 4 shows the Figure of Merit's components. The 2006-2012 reference change is 349 the union of Misses, Hits, and Wrong Hits. The 2006-2012 simulation change is the union of 350 Hits, Wrong Hits and False Alarms. The CA-Markov model allocated the gain of each category around patches of the category at 2006, which caused long winding patches of simulation 351 352 change. The shapes of the patches of simulation change do not match the compact and isolated 353 patches of reference change. Correctly simulated persistence accounts for 97% of the spatial 354 extent, which is why overall percent correct and kappa at the end time point are misleading 355 measurements of a model's ability to simulate change.



356 357 Figure 4 Three-map comparison to examine simulation versus reference change during 2006-358 2012. The numbered boxes show three regions that contain Hits.

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367

360 The Figure of Merit is 0.07%, which is the size of Hits as a percentage of the sum of sizes of the four components. Figure 5 shows that Hits accounted for 0.02% of the spatial extent. 361 362 Reference change during 2006-2012 accounted for 1.12% of the spatial extent, which is the sum of Misses, Hits, and Wrong Hits. Simulation change accounted for 1.53% of the spatial 363 364 extent, which is the sum of Hits, Wrong Hits and False Alarms. Quantity disagreement is 0.41% 365 while allocation disagreement is 2.12 % of the spatial extent. Total disagreement is 2.57%, 366 which is the sum of Misses, Wrong Hits and False Alarms.





369

4 Discussion

371 4.1 Quantity Disagreement and Intensity Analysis

The CA-Markov model uses a Markov chain to guide the simulation's quantity of each transition. Intensity Analysis shows how the simulation produced small differences with respect to 2006-2012 reference concerning quantity.

375 Intensity Analysis' interval level showed that the model simulated correctly the 376 deceleration of overall change from the calibration interval to the validation interval. Many 377 Markov chains lead to a steady state concerning the size of each category, in which case the 378 Markov chain extrapolates a deceleration of change. Intensity Analysis' category level showed 379 that the Markov algorithm simulated the dormant or active status of each category's loss and 380 gain as the category's same status during the calibration interval. Intensity Analysis' transition 381 level showed that the simulated gain of Artificial targeted Agriculture, as was the case during 382 the calibration interval; however, the reference gain of Artificial targeted Forest during the 383 validation interval. The simulation did not match the reference pattern during the validation 384 interval because the reference pattern was not stationary concerning transitions to Artificial. 385 Intensity Analysis' transition level showed that the simulated gain of Forest targeted 386 Agriculture and Wetland, which is a pattern that was stationary through time according to the 387 reference data.

Additional analysis showed that Idrisi Selva's CA-Markov model simulated fewer and smaller transitions than an extrapolation of a Markov chain would dictate. Table 3 shows that Artificial experienced loss and Wetland experienced gain during the calibration interval, but the CA-Markov model simulated zero loss of Artificial and zero gain of Wetland. This illustrates how the CA-Markov did not follow the quantities that a pure Markov extrapolation would have dictated.

394

395 4.2 Allocation Disagreement and Figure of Merit's Components

The CA-Markov model uses the Cellular Automata algorithm primarily to guide the change's allocation. FOM's components showed how the simulation had substantial differences related to the 2006-2012 reference concerning allocation.

399 Hits and Wrong Hits were near zero, which indicates that the simulation change did not 400 correspond to the reference change. If Misses or False Alarms equal zero, then allocation 401 difference is zero. If Misses equal False Alarms, then quantity difference is zero. If Misses are 402 greater than False Alarms, then reference change is greater than simulated change. If Misses 403 are less than False Alarms, then reference change is less than simulated change, which our case 404 study illustrates. In our application, the sizes of Misses and False Alarms imply that allocation 405 difference was greater than quantity difference. This implies that disagreement during the 406 validation interval derived more from the model's Cellular Automata algorithm than from its 407 Markov algorithm.

408 If we had examined only the single FOM metric, then we would not be able to have the 409 insights that we had from interpretation of Misses, Hits, Wrong Hits and False Alarms. FOM's 410 single number combines quantity disagreement and allocation disagreement into one 411 measurement, which fails to reveal whether disagreement derives from quantity or allocation. 412 If the quantity of simulation change differs substantially from the quantity of reference change 413 during the validation interval, then it is possible for FOM to be small, even when the simulation 414 allocates change as accurately as possible. For example, if the simulation change is a small 415 subset of the reference change, then then FOM will be small, even when False Alarms are zero. 416 If the reference change is a small subset of the simulation change, then the FOM will be small, 417 even when Misses are zero. FOM's components reveal the reasons for the size of the FOM.

In our application, the Cellular Automata algorithm did not use the 2000-2006 reference change to calibrate the allocation of simulated change. The algorithm's spatial filter causes a category to gain around the edges of the category's patches. However, figure 1 shows that reference change in our study area is rarely allocated around the edges of patches. Our use of the spatial filter may be one reason for the large allocation disagreement.

423 We performed sensitivity analysis to see how the size of the spatial filter influences the 424 results. We ran the model with spatial filters of 3-by-3, 5-by-5 and 7-by-7. Output showed trivial 425 variation in the simulation. The variation of the spatial filter caused variation in the quantity of 426 change for at most 36 cells of simulation loss of Wetland. Figure of Merit was 1.6% for 3-by-427 3, 0.7% for 5-by-5 and 0.6% for 7-by-7. All three sizes of the spatial filter cause simulated 428 change to occur near patch edges, whereas a larger spatial filter allows change to occur slightly 429 farther from patch edges. The sensitivity results suggest that reference change is slightly more 430 concentrated directly adjacent to patch edges in the rare cases where reference change exists 431 near patch edges. Increase of the iteration parameter from six to twelve caused FOM values to 432 shrink. More sophisticated sensitivity analysis for model parameters is a topic for future 433 research (Saltelli et al. 2008).

Some investigators have compared CA-Markov model runs that used a spatial filter to
runs that did not use a spatial filter (Camacho Olmedo et al. 2015; Pontius and Malanson 2005).
They found that the spatial filter influenced the simulation's allocation, but did not influence
Hits substantially.

438 Another possible reason for the large allocation disagreement might be that we did not 439 use suitability maps to guide the spatial allocation. Idrisi's CA-Markov allows inclusion of 440 suitability maps that use independent variables for calibration. We did not use such suitability 441 maps because our purpose was to show methods for model assessment. Other authors used 442 suitability maps in their applications, while they saw results similar to ours concerning 443 allocation disagreement (Memarian et al. 2012; Pontius Jr et al. 2008; Pontius Jr et al. 2011) 444 Even if we were to have used suitability maps, the CA's spatial filter would have still caused a 445 category to gain around the category's existing patches. If the reference maps do not show 446 spatial dependency and the goal is predictive power, then the modeler should not use a spatial 447 filter.

448 Some modellers are tempted to modify the simulation model in an effort to increase 449 accuracy. A modeller should first have a specific goal for a particular validation metric before 450 modifying the model. The goal will help the modeler to decide where to focus attention. Deep 451 thought is necessary to select a relevant validation metric and a goal for the metric. The modeller 452 must consider the particular applied research question to select the metric and its goal. In our application to Hungary, the size of simulation change was 1.53% of the spatial extent and the 453 454 reference change was 1.12%. If the main goal is to simulate the quantity of change, then perhaps 455 the simulation of somewhat more than the reference change is tolerable, while allocation 456 difference is less important. For example, if the goal is to simulate disturbance of carbon in a 457 region where carbon density is spatially uniform, then quantity difference determines error of 458 carbon disturbance, while allocation difference is irrelevant (Pontius 2018). However, if carbon 459 density is not spatially uniform, then allocation difference can be important for simulation of 460 carbon disturbance. Modellers must consider the goal of the simulation before jumping to an 461 endless chase to increase accuracy. This article gives metrics to help modelers align the goal of 462 the simulation with various aspects of the model. For this article's Hungarian example, validation results showed allocation disagreement is much larger than quantity disagreement. 463 464 So if the goal is to decrease total disagreement, then the modeler should focus on the allocation of change. The first step would be to simplify the CA-Markov model by eliminating the spatial 465 filter, because the reference change is not concentrated near patch edges. The second step would 466

467 be to use suitability maps to guide the allocation of simulated change. Idrisi's CA-Markov468 model has the ability to include such suitability maps.

469

470 4.3 Limitations and Pitfalls of Popular Metrics

471 Some scientists aim to use a single metric to evaluate modelling applications. However, 472 any single metric cannot offer insights concerning various aspects of modelling applications. 473 For example, a popular and misleading metric is the percent correct between the simulation 474 map and the reference map at the end time point of the validation interval (Kityuttachai et al. 475 2013). Our application was 97% correct according to a two-map comparison between the 476 simulation and the reference maps at 2012. Persistence simulated correctly is the reason for the 477 large percent correct. Percent correct at the validation interval's end time point fails to 478 distinguish between correctly simulated persistence versus correctly simulated change. Clear 479 interpretation is limited or impossible for some other popular metrics, such as FOM and the 480 kappa index of agreement (Yang et al. 2014; Subedi et al. 2013; Parsa et al. 2016; Chakraborti 481 et al. 2018). Scientists claim kappa is an index that accounts for random agreement. But kappa 482 accounts for randomness in a confusing, misleading and irrelevant manner (Pontius Jr and 483 Millones 2011). Furthermore, kappa is not appropriate for validation of temporal change 484 because kappa compares two maps at a single time point, thus cannot give insight concerning 485 temporal change. The FOM examines temporal change during the validation interval, but the 486 FOM offers limited interpretation because the FOM combines quantity disagreement and 487 allocation disagreement into a single metric. A metric that combines various concepts can be 488 difficult to interpret (Bradley et al. 2016). It is more helpful to use a collection of metrics, where 489 each metric reveals a distinct and clear aspect of the modelling application. Furthermore, we 490 recommend authors show maps that reveal reference change during the calibration interval, 491 simulation change during the validation interval, and reference change during the validation 492 interval. An overlay of the latter two maps show Misses, Hits, Wrong Hits, False Alarms and 493 Correct Rejections, which communicates clearly the quantity and allocation of changes during 494 the validation interval (Shafizadeh-Moghadam et al. 2017).

495

496 **5 Conclusions**

497 We have presented novel methods to interpret applications of land change models. Our 498 collection of metrics reveals various aspects that are helpful to understand simulations of 499 temporal change. For our CA-Markov modelling application for a Hungarian case study, 500 Intensity Analysis' interval level shows the model simulated more change than the reference 501 change during the validation interval, because the reference change decelerated from the calibration interval to the validation interval. Intensity Analysis' category level shows the CA-502 503 Markov model did not follow exactly the loss intensities that a pure Markov chain would imply. 504 Intensity Analysis' transition level shows the model simulated correctly that the gain of Forest 505 targeted Agriculture and Wetland. Hits were almost zero, which indicates almost no intersection 506 between simulated and reference change during the validation interval. Misses and False 507 Alarms showed that allocation difference was larger than quantity difference, which reflects 508 how the Cellular Automata algorithm caused more error than the Markov algorithm.

509 We conclude with recommendations that apply generally. Scientists must compare 510 visually and quantitatively the changes during three intervals: (i) reference change during the calibration interval, (ii) simulation change during the validation interval, and (iii) reference 511 512 change during the validation interval. Comparison between (i) and (ii) relates the calibration 513 patterns to the subsequent simulation. Comparison between (ii) and (iii) distinguishes between simulation and reference changes during the validation interval. Comparison between (i) and 514 515 (iii) shows the degree to which the reference patterns are stationary through time. For each 516 comparison, Intensity Analysis reveals various levels of information concerning quantity

- 517 disagreement. The FOM's components distinguish quantity disagreement from allocation
- 518 disagreement during the validation interval. Our recommended collection of metrics generate
- 519 insights that are deeper than any single metric can communicate.
- 520

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