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The Complexities of Agent-Based Modeling Output Analysis

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Abstract

The proliferation of agent-based models (ABMs) in recent decades has motivated model practitioners to improve the transparency, replicability, and trust in results derived from ABMs. The complexity of ABMs has risen in stride with advances in computing power and resources, resulting in larger models with complex interactions and learning and whose outputs are often high-dimensional and require sophisticated analytical approaches. Similarly, the increasing use of data and dynamics in ABMs has further enhanced the complexity of their outputs. In this article, we offer an overview of the state-of-the-art approaches in analysing and reporting ABM outputs highlighting challenges and outstanding issues. In particular, we examine issues surrounding variance stability (in connection with determination of appropriate number of runs and hypothesis testing), sensitivity analysis, spatio-temporal analysis, visualization, and effective communication of all these to non-technical audiences, such as various stakeholders.

Keywords:
Agent-Based Modelling, Methodologies, Statistical Test, Sensitivity Analysis, Spatio-Temporal Heterogeneity, Visualization

Introduction

1.1 Agent-based models (ABMs) have been gaining popularity across disciplines and have become increasingly sophisticated. The last two decades have seen excellent examples of ABM applications in a broad spectrum of disciplines including ecology (Grimm & Railsback 2005; Thiele & Grimm 2010), economics (Kirman 1992; Tesfatsion & Judd 2006), health care (Effken et al. 2012), sociology (Macy & Willer 2002; Squazzoni 2012), geography (Brown & Robinson 2006), anthropology (Axelrod & Hammond 2003), archaeology (Axtell et al. 2002), bio-terrorism (Carley et al. 2006), business (North & Macal 2007), education (Abrahamson et al. 2007), medical research (An & Wilensky 2009), military tactics (Ilachinski 2000), neuroscience (Wang et al. 2008), political science (Epstein 2002), urban development and land use (Brown et al. 2005), and zoology (Bryson et al. 2007). This methodology now also penetrates organizational studies (Carley & Lee 1998; Lee & Carley 2004; Chang & Harrington 2006), governance (Ghorbani et al. 2013), and is becoming actively employed in psychology and other behavioural studies, exploiting data from laboratory experiments and surveys (Duffy 2006; Contini et al. 2007; Klingert & Meyer 2012).

1.2 ABMs produce a rich set of multidimensional data on macro phenomena, comprising a myriad of details on micro-level agent choices and their dynamic interactions at various temporal and spatial resolutions. Despite significant progress made in empirically grounding ABM mechanisms and agent attributes (Robinson et al. 2007; Windrum et al. 2007; Smajgl et al. 2011), ABMs continue to harbour a considerable amount of subjectivity and hence degrees of freedom in the structure and intensity of agents' interactions, agents' learning and adaptation, and any potential thresholds affecting switching in strategies. The increasing complexity of ABMs has been further stimulated by improvements in computing technology and wider availability of

advanced computing resources. These qualities demand a comprehensive (or at least sufficient) exploration of the model's behaviour.

1.3 To complicate matters further, an ABM is typically a *stochastic* process and thus requires Monte Carlo sampling, in which each experiment (or parameter setting) is multiply performed using distinct pseudo-random sequences (i.e., different random seeds) in order to achieve the statistical robustness necessary for testing hypotheses and distinguishing multiple scenarios under varying experimental or parameter settings. By "random seed", we mean the seed for the random number generator. Thus, an ABM delivers a high volume of output data rendering the identification of salient and relevant results (such as trends) and the assessment of model sensitivities to varying experimental conditions a challenging problem.

1.4 All these complications apply not only to the analysis of ABM output data but also to the model's design and implementation. The massive diversity in outputs, often exhibiting temporal and spatial dimensions, necessitates judicious model design, planning, and application. Poor or unstructured design may lead to unnecessarily larger outputs to reach the same (or even less) precise conclusions that one may infer from outputs of well-designed models and experimentation. The standards employed in the ABM field, such as ODD (Overview, Design concepts, and Details) (Grimm et al. 2006, 2010; Müller et al. 2013) and DOE (design of experiments) (Fisher 1971), have significantly improved transparency, replicability, and trust in ABM results. However, the field continues to lack specific guidance on effective presentation and analysis of ABM output data, perhaps due to this issue's having less priority in ABM social science research or due to technical barriers. Furthermore, converging on universal standards remains elusive partly due to the broad spectrum of research fields employing ABMs. Domain-relevant metrics, analytical techniques, and communication styles are largely driven by each discipline's target audience.

1.5 Yet, there are common methodological challenges facing ABM modellers in their path toward understanding, refining, and distilling the most relevant and interesting results from a nearly-endless sea of output data. While a modeller invests a significant amount of time and effort in the development of an ABM itself, a comprehensive or compelling analysis of the ABM output data is not always considered as deserving the same resource-intensive attention. Proper output analysis and presentation are vital for developing a domain-specific message containing innovative contributions.

1.6 This paper aims to provide an overview of the state-of-the-art in how agent-based modellers contend with their model outputs, their statistical analysis, and visualization techniques.[1] We discuss challenges and offer examples for addressing them. The first topic deals with several issues surrounding the study of variance in the model outputs (i.e., stability) and its impact on both model design (e.g., simulation runs or "samples") and analysis (e.g., hypothesis testing). The next one addresses the state of sensitivity analysis and the complexities inherent in the exploration of the space that encapsulates both the parameters and the outcomes. The third topic focuses on the analysis and presentation of spatial (including geospatial) and temporal results from ABMs.

1.7 We also survey the role of effective visualization as a medium for both analysis and exposition of model dynamics. Comments on visualization appear within each main topic as visualization strategies tend to be strongly defined and constrained by the topic matter. Finally, we outline outstanding issues and potential solutions which are deemed as future work for ourselves and other researchers.

Determining Minimum Simulation Runs and Issues of Hypothesis Testing

2.1 ABM researchers strive to expose important and relevant elements in their models' outputs and consequently the underlying complex dynamics in both quantitative and qualitative ways. Compelling statements about an ABM's behaviours may be drawn from descriptive statistics of distinct outcomes (e.g., mean and standard deviation) or statistical tests in which outcomes are compared (e.g., *t*-test), predicted (in the statistical sense, e.g., multiple regression), or classified (e.g., clustering or principal component analysis). Given the stochastic nature of most ABMs, these analytical exercises require an outcome pool drawn from a sufficient number of samples (i.e., simulation runs).

2.2 The quantity of ABM output samples has several ramifications to experimental design and the quality of the analysis. For those large and complex ABMs whose longer run times prohibit the production of large samples, the relevant question is the minimum number of required runs. Conversely, expedient ABMs offer the temptation of producing far greater sample counts thereby increasing the sensitivity of statistical tests possibly to the point of absurdity. That is, one might produce so many samples such that traditional tests expose extremely small and contextually inconsequential differences. We focus our discussion on the methods for the determining the number of minimum runs. Implications of having too many samples are discussed in Appendix B.

Minimum Sample Size (Number of Runs)

2.3 The determination of the minimum sample size partly relies on the analytical objective. One common objective is a statistical description of the outcomes typically in the form of means and standard deviations (or alternatively, variances). Since the shape of a model's output distributions are usually *a priori* unknown, the point or sample size at which outcome mean and variance reaches relative quiescence or stability is crucial to accurate reporting of the descriptive statistics. Otherwise, the statistics would harbour too much uncertainty to be reliable. Unfortunately, all of the different criteria for determining this point of stability suffers from some degree of subjectivity, and thus it falls on the analyst to wisely make the selection. Furthermore, these approaches appear to remain either underused or unknown to many ABM researchers (Hamill 2010). In fact, a survey of some of ABM literature reveals sample sizes to be too low, conveniently selected (sample sizes of 100 or less are common), or exorbitantly

high (Angus & Hassani-Mahmooei 2015).

Variance Stability

2.4 Assessing variance stability requires a metric to measure the uncertainty surrounding the variance (or the variance of variance if you will). Law and Kelton (2007) and Lorscheid et al. (2012) offer such metrics both of which rely on some functional ratio between the variance and the sample mean. Law & Kelton's approach seeks a sample size in which the variability remains within some predefined proportion of the confidence interval around the mean (*confidence interval bound variance*), thus it is bound to the assumptions of normality, namely that the mean has a Gaussian distribution. Hence, the researcher must select this proportion from outputs of a trial set of runs. Lorscheid et al.'s method eschews those assumptions by employing the *coefficient of variation* and a fixed *epsilon* (E) limit of that metric. While these are dimensionless metrics, their use is problematic for simulation studies in which multivariate outcomes from parameter effects are analyzed.

2.5 The coefficient of variation is simply the ratio of the standard deviation of a sample (σ) to its mean (μ):

$$c_V = \frac{\sigma}{\mu}$$

2.6 This scaling offers a similar interpretation as the confidence interval (C.I.): $c_V \to 0$ is equivalent to $t(0 \notin \text{C. I.}) \to \infty$ and the p-value approaches 0. That is, when the standard deviation shrinks relative to the mean, the probability of the confidence interval spanning across the value of 0 drops precipitously. The coefficient of variation (c_V) will exhibit substantial variance for small sample sizes just like the standard error of the mean. For example, the c_V of a single ABM outcome obtained from a set of five runs will vary more with the same metrics taken from other sets of five runs than if each set contained far more runs, say 100. Lorscheid et al. compare the c_V's of differently sized sets of runs (e.g., the c_V from 10 runs, then 100, 500, and so forth). The sample size at which the difference between consecutive c_V's falls below a criterion, E, and remains so is considered a minimum sample size or minimum number of ABM runs. For example, if an outcome drawn from runs of different sample sizes, $n \in \{10, 500, 1000, 5000, 10000\}$, yields the c_V's (rounded to 1/100) $\{0.42, 0.28, 0.21, 0.21, 0.21\}$ and we select $E = 0.01$, we would consider the third sample size ($n = 1000$) as the point of stability. These c_V stability points are obtained for all ABM outcomes of interest (in a multivariate setting), and thus the minimum number of runs for the ABM is the maximum of these points:

$$n_{\min} = \text{argmax}_n |c_V^{x,n} - c_V^{x,m}| < E, \ \forall x \text{ and } \forall m > n$$

where $n_{\min}$ is the estimated minimum sample size; x is a distinct outcome of interest; and m is some sample size $> n$ for which the c_V (of each outcome) is measured.

2.7 However, the fixed E favors those μ sufficiently larger than 0 and also larger than its corresponding σ and penalizes $n_{\min}$ for outcomes with μ closer to 0. That is, the more likely an outcome's confidence interval encompasses 0, the erroneously larger the estimation of $n_{\min}$ will be. Conversely, the fixed E renders the procedure too effective and results in an underestimation of $n_{\min}$ for those C.I.'s that reside far from 0, relative to σ. Therefore, we urge some caution in using c_V to determine the minimum sample size and applying it only to ABMs for which the outcomes of interest are prejudiced against attaining a value of 0. As such, Lorscheid et al.'s approach determines a minimum sample size not just based on variance stability but also the likelihood an outcome's confidence interval contains 0.

2.8 Alternatively, one might consider just variance stability without any consideration of the mean value. Following Lorscheid et al.'s strategy of assessing stability from metrics on an outcome for a sequence of sample sizes, we track the *windowed variance* of simple outcomes from several canonical statistical distributions as well as an ABM model. The distributions we employ here for demonstration purposes are the normal (or Gaussian), uniform, exponential, Poisson, χ^2, and t distributions.[2] While ABM outputs do not always conform to one of these parametric distributions, the ones we examine here are distinct enough to provide us with a sense of variance stability for a spectrum of distributions. These distributions will serve as proxies for ABMs' outcomes and, for our purposes, have been parameterized so that their theoretical variance $\sigma^2 \approx 1$. We also include an outcome from a simple ABM model of Birth Rates (Wilensky 1997). This ABM entails two dynamically changing populations (labelled "red" and "blue"). Here, our outcome is the size of the "red" population. For further details, see Figure 17 in Appendix C.

2.9 In Figure 1a, we offer variances for varying sized samples of Gaussian variates (i.e., scalars drawn from the Gaussian distribution parameterized to have a variance of 1). At low sample sizes, there is considerable variance surrounding the sample variance itself as evidenced by the "noisiness" of the variance from one sample size to the next. After a certain point (roughly $n = 400$), this *outer variance* appears to stabilize and continues to further converge to 0 albeit slowly.

2.10 The outer variance at each sample size can then be measured using the variance of proximal sample sizes. For example, the outer variance for $n = 10$ is calculated from variance of the sample variances of $n \in \{10, \ldots, 10 + (W-1)g\}$, where W is some

predetermined size of the window and g is our sample size increment; we select $g = W = 10$, and we so consider $n \in \{10, 20, \ldots, 100\}$ for the variance surrounding $n = 10$. Notationally, this outer variance may be expressed as σ^2 (s^2) but given its estimation using windows, we assign it ω_n^2, where n is the sample size. In Figure 1, we chart the ω_n^2 relative to its maximum value ($\frac{\omega_n^2}{\max\omega^2}$) for each distribution.

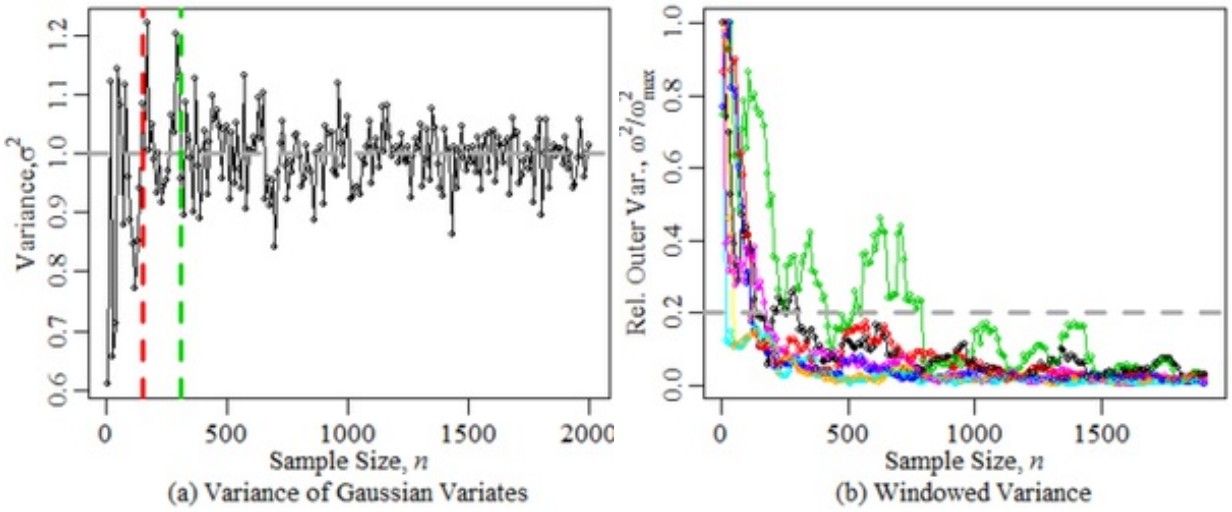


Figure 1. Sample Size vs. Variance Stability. *The colours in the right plot denote the distribution: normal, uniform, exponential, Poisson, χ^2, Student's t, and Birth Rate ABM.*

2.11 The colours distinguish the seven distributions. The grey, dashed horizontal line expresses our semi-subjective criterion (of 0.20) under which the relative ω_n^2 must reside in order for n to be deemed a "minimum sample size". The speed at which this condition is met varies considerably among the distributions, highlighting the need to forego distributional assumptions regarding ones ABM outputs in variance-based minimum sample size determination, unless the distributional shapes are well-identified. This approach for assessing variance stability bears two elements of further subjectivity. Firstly, the point of stability may be identified by either the first n at which the criterion condition is met or the first n at which all further sample sizes meet the condition. The red and green vertical lines in Figure 1a respectively denote these points of stability for the Gaussian distribution. Secondly, the outer variance could have been assessed using a larger pool of variates at each n rather than estimated under windows. However, in keeping with the strategy of minimizing the number of test simulation runs $n_{\min}$, we report the findings of window-based ω^2 rather than σ^2 (s^2).

Effect Size

2.12 In traditional statistical analysis, the common approach for determining minimum sample size requires one to first select the size of a detectable effect (i.e., a statistic such as the mean or difference of means scaled by a pooled standard deviation). This approach also requires a selection of acceptable levels of the *type I* and *type II* errors. A type I error is coarsely the probability (in the frequentist sense) that the null hypothesis is rejected when in fact it is true. The type II error is the converse: the likelihood that the null hypothesis is retained when the alternative hypothesis is true. For example, one might compare the means of two ABM outcomes each from separate sets of sample of runs. These outcomes may be borne of distinct model parameterizations (a necessary though not sufficient condition for yielding a true difference) and measured to be significantly different under a rudimentary *t-test*. However, a small sample size will penalize the test which may not report a statistically significant difference between means of those outcomes: a type II error. Alternatively, these outcomes may arise from identical parameterizations yet the *t*-test erroneously reveals a significant difference: a type I error. The rates of type I and II errors are expressed as α and β. The converse of the type II error ($1-\beta$) is called the "power" level.

2.13 The minimum sample size $n_{\min}$ can then be computed as

$$n_{\min} \geq 2\frac{s^2}{\delta}(t_{V,1-\alpha/2} + t_{V,1-\beta/2})^2$$

where s is the standard deviation of the outcome or the pooled standard deviation of two outcomes, δ is lower bound on the absolute difference in means that is to be classified as significantly different; t is the *t*-statistic (or the quantile function of the *t* distribution); v is the degrees of freedom (here $n_{\min} - 1$), and α and β are the levels of type I and II errors respectively. In lay terms, the minimum sample size occurs at the point at which both type I and type II errors occur at the desired *critical levels* as determined by the *t*-test, hence the employment of the *t* distribution. This approach has been suggested in the ABM literature (e.g., Radax & Rengs 2010). As $n_{\min}$ appears on both sides of the equation, trial-and-error or algorithmic iterations can usually

converge on $n_{\min}$. A similar equation is employed when the outcome is a proportion $\in [0, 1]$. The non-central *t* distribution can also be used for sample size determination (as in the R statistical package).

2.14 A close inspection of this approach reveals test sensitivity to the outcome distribution's departure from the normal. In Table 1, we empirically measure the power level (and hence the level of type II error) by drawing pairs of variate sets from some typical distributions and the Birth Rate model, parameterized such that identical effect sizes of 0.5.[3] Thus, an insignificant *t*-test comparison for a pair of variate sets is tantamount to a type II error. For each distribution type and sample size n, the comparison was performed for 5000 pairs of variate sets each of size n. Each set pair was compared, and we monitor the proportion of pairs of these sets that yielded a significant p-value: an empirically-derived power level. The empirical power levels for a range of sample sizes n are graphically shown in Figures 15 and 16 in Appendix A.

Table 1: Minimum Sample Sizes for Outcome Distributions. n_t, n_e, *and* n_W *are the theoretically-derived, empirically-derived, and Wilcox-test-based minimum sample sizes,* $n_{\min}$.

Distr.	n_t	n_e	n_W	$n_e - n_t$	$n_W - n_t$
Normal	64	65	68	1	4
Exponential	64	59	78	-5	14
Poisson	65	61	64	-4	-1
Birth Rate	64	65	70	1	6
Birth Rate ($d = 1.0$)	18	19	26	1	8

2.15 We observe incongruities between the theoretical $n_{\min}$ (n_t) and the empirically-derived n_e. In fact, the power calculation overestimates $n_{\min}$ for the skewed distributions (i.e., the exponential and the Poisson). While the differences in these $n_{\min}$ are relatively minor, they could have a material benefit for large scale ABMs for which each run is costly. However, in these cases, using the *t*- test for exposing a predetermined effect size has to be deemed appropriate. For these surveyed distribution types, the empirical distributions of the means themselves frequently pass the Shapiro test of normality hence allowing for the use of the *t*-test.

2.16 Given the sensitivity of the traditional *t*-test to distributional skewness as well as the uncertainty of the distributional shape in ABM outcomes, one might turn to a more conservative test, the *Wilcoxon ranked sum test* (also known as the *Mann-Whitney test*); the n_W column reports this test's suggested minimum sample sizes. Interestingly, the more efficient Wilcoxon test appears to propose a lower minimum size for the Poisson distribution.

2.17 When we assess the efficiency of calculating $n_{\min}$ for the Birth Rate ABM, we find that, despite the flatness plus bimodality of the outcome distribution, the calculation of $n_{\min}$ is almost accurate, and the Wilcox test is modestly conservative compared to the exponential distribution.

Multivariate Stability

2.18 Since most ABMs typically produce multiple outcomes, the calculation of the required sample size would have to consider all outcomes of interest. Furthermore, analysis of ABMs often entails an exploration of parameter settings (or the parameter space) in order to understand the dependencies between key input parameters and their outcomes including their variability. Given the complexity of ABMs, the outcomes' variance may or may not be constant (i.e., homoskedastic) across the parameter settings. Hence, the task of understanding model output sensitivity to different experimental conditions that are relevant to the research question is vital. While the topic of sensitivity analysis is further elaborated in 3.1, we discuss it here briefly given its role in determining the adequate run sample size applicable to all the chosen parameter settings. Well-structured DOE (described further in Section 3) can be very helpful to comprehensively explore model variabilities corresponding to multiple model parameters.

Visualization for statistical issues

2.19 One visualization approach for examining univariate ABM outcome distributions is the *violin plot* which combines elements of a box plot and a kernel density plot, with a smoothed estimation of outcomes' variances across the ranges of factors/parameters (see, e.g., Kahl & Hansen 2015). Figure 2 illustrates the multifaceted influence of six variables (each with 3 values following a 3^k factorial design) on the output measure ("compensation payment"). Details may be found in Lorscheid (2014).

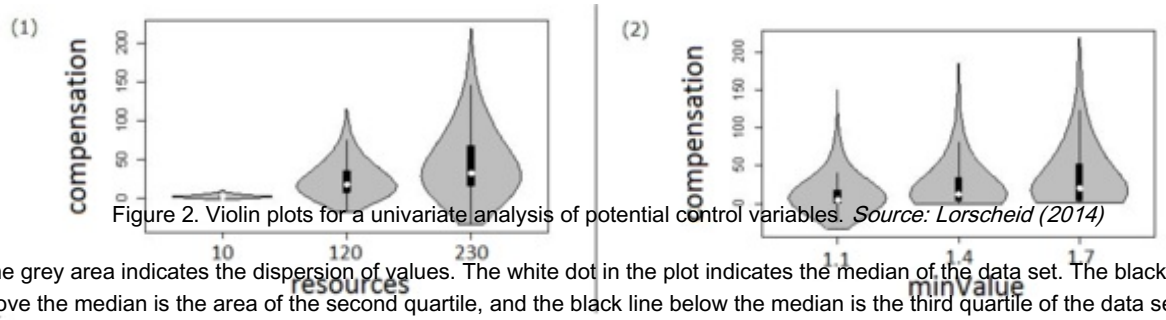


Figure 2. Violin plots for a univariate analysis of potential control variables. *Source: Lorscheid (2014)*

2.20 The grey area indicates the dispersion of values. The white dot in the plot indicates the median of the data set. The black line above the median is the area of the second quartile, and the black line below the median is the third quartile of the data set. For a detailed description of violin plots see Hintze and Nelson (1998).

Solution space exploration and sensitivity analysis

3.1 There are a variety of topics that may be gathered under the broad heading of parameter or input-output space exploration, including optimization, calibration, uncertainty analysis, sensitivity analysis, as well as the search for specific qualitative model features such as "regime shifts" and "tipping points". In all cases, the goal is to provide additional insight into the behaviour of the ABM through the examination of certain parameter settings and their corresponding output measures.

3.2 We will first discuss "exploration" in a broad sense, followed by a more detailed discussion of a variety of methods for performing one particularly important exploration task: sensitivity analysis.

Input/Output Solution Space Exploration

3.3 One of the most common forms of parameter space exploration is *manual* (or *human-guided*) *exploration* (also called the "trial-and-error method" or "educated guessing"). This approach can be computationally efficient if guided by an individual familiar with the model's dynamics and/or outputs. The intuitions of a model's author/developer, a domain expert, or a stakeholder can inform parsimonious, iterative parameter selection in such a way as to generate and test relevant hypotheses and minimize the number of regions searched or the number of required simulation runs. However, this exploration strategy is vulnerable to human bias and fatigue leading to a disproportionate amount of attention paid to the target phenomena and the neglect of large portions of the model's behaviour space. Distributing the burden of the exploration task (e.g., crowd sourcing) may address some of its limitations. Nevertheless, more systematic, automated, and unbiased approaches are required to complement the shortcomings of solely human-guided searching, which will always play a role in space exploration, especially in its preliminary stages.

3.4 The simplest of the systematic exploration approaches fall under the class of *regular sampling techniques* in which the parameters are chosen (or sampled) in a systematic manner to ensure their having certain statistical or structural properties. Some of these techniques are *random*, *quasirandom*, *gridded/factorial*, *Latin hypercube*, and *sphere-packing*. Sampling may globally consider the entire parameter space or focus locally on a particular region (e.g., altering one parameter at a time for "univariate sensitivity analysis"). The well-established methodological history of DOE and the recent literature on design and analysis of simulation experiments (e.g., Sacks et al. 1989) can guide the sampling strategy. However, the complexity of ABMs (and their outputs) can render classic DOE inappropriate as noted by Sanchez and Lucas (2002). Classic DOE (a) assumes only linear or low-order interactions among experimental parameters (or factors) and outputs, (b) makes little or no provision for the iterative parameter selection process (i.e., sequential virtual experiments), and (c) also assumes typical error (Gaussian and unimodal) in the output. An example of multi-modal ABM output is presented in Appendix C. Thus, traditional DOE methods, while useful for ABMs, ought to be implemented with caution and consideration for appropriate methods that address complexities in the output. Research into DOE methods for ABMs is still evolving (Klein et al. 2005; Kleijnen et al. 2005; Ankenman et al. 2008; Lorscheid et al. 2012).

3.5 Research into more sophisticated exploration techniques has been informed by *meta-heuristic searching*, *optimization algorithms*, and *machine learning*. Researchers propose the use of genetic algorithms (GA) (Holland 1975) for a wide range of exploration tasks including directed searches for parameters that yield specific emergent behaviours (Stonedahl & Wilensky 2011), parameter optimization (Stonedahl et al. 2010), calibration/parameter estimation (Calvez & Hutzler 2006; Heppenstall et al. 2007; Stonedahl & Rand 2014) and sensitivity analysis (Stonedahl & Wilensky 2010). The *query-based model exploration* (QBME) paradigm provided by Stonedahl and Wilensky (2011) expands Miller's (1998) application of GA in ABM output exploration. In QBME, parameters producing user-specified model behaviours are discovered through automation such as GAs, thus inverting the traditional workflow (see Figure 3). Stonedahl and Wilensky (2011) demonstrate QBME for identifying convergence, divergence, temporal volatility, and geometric formations in models of collective animal motion (i.e., flocking/swarming).

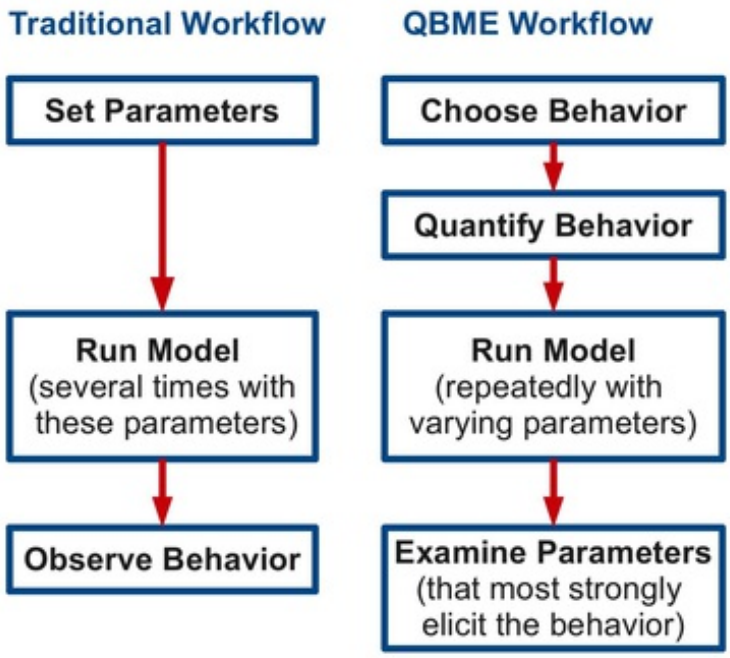


Figure 3. Query-Based Model Exploration (QBME). *This framework for exploring ABM parameter-spaces exploits genetic algorithms (or other meta-heuristic search algorithms) to efficiently search for parameters that yield a desired model behaviour. Source: Stonedahl and Wilensky (2011)*

Sensitivity analysis: Approaches and challenges

3.6 *Sensitivity analysis* (SA) is a variation of parameter/input-output space exploration that focuses on model response to changes in the input parameters (Figure 4). Specifically, the researcher seeks to identify parameters for which small variations most impact the model's output.

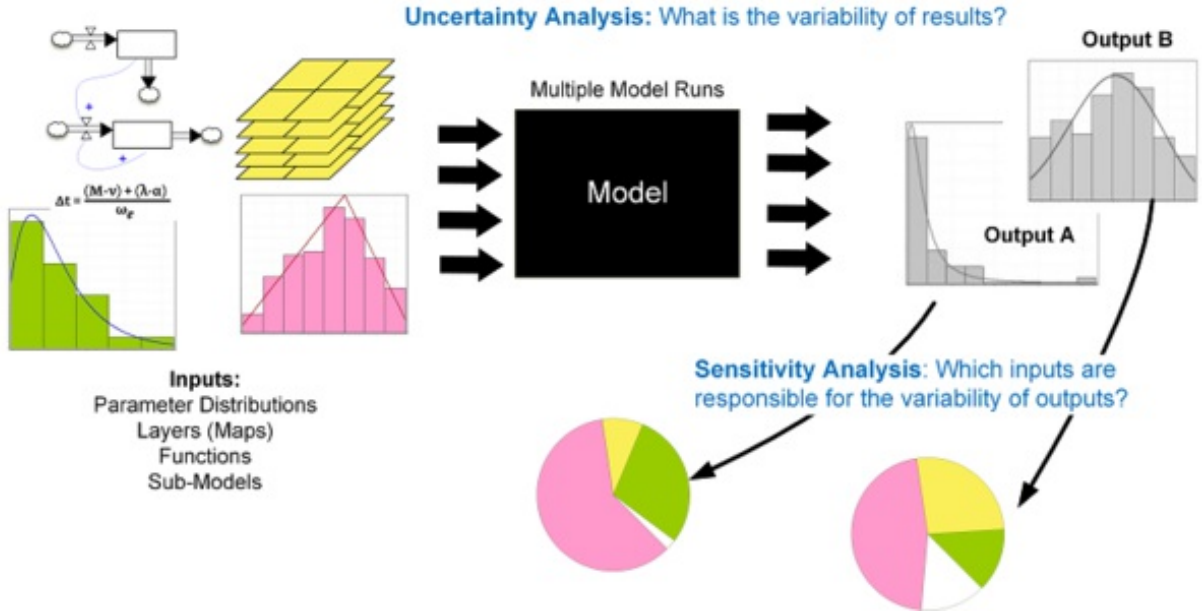


Figure 4. Uncertainty and sensitivity analysis as part of the modelling process. Source: Ligmann-Zielinska et al. (2014)

3.7 This discovery can aid in prioritizing prospective data collection leading to improved model accuracy, reduction of output variance, and model simplification (Ligmann-Zielinska et al. 2014). Model insensitive parameters may even be relegated to mere numerical constants thereby reducing the dimensionality of the input parameter space and promoting model parsimony; this simplification process is referred to as "factor fixing" (Saltelli et al. 2008). Ignoring these non-influential input parameters can have ill-effects on the model by increasing its computational cost and also on its reception when these parameters are controversial for stakeholders not involved with the model's development (Saltelli et al. 2008).

3.8 The proliferation of various SA methods stems from the variety of ABM styles and research problems ABMs address as well as from the availability of increasing computational capacity (Hamby 1994; Saltelli et al. 2000). Currently, the ABM practice of SA has entailed one or more of the following methods: *one-parameter-at-a-time*, *elementary effects*, *standardized regression coefficients*, *meta-modelling*, and *variance-based decomposition* (Thiele et al. 2014; ten Broeke et al. 2014). Below, we briefly

discuss each of these, their advantages, and drawbacks, in the context of ABMs.

3.9 In *one-parameter-at-a-time* (OAT), each input parameter in turn is examined over a set of values (defined either *ex ante* to the SA or dynamically during SA) and in isolation by holding the other parameters at a constant baseline. Meanwhile, the effects of these marginal (i.e., one-at-at-time) parameter changes are monitored, and repeated iterations increase the procedure's robustness. Hassani-Mahmooei and Parris (2013), for example, applied OAT to their ABM of micro-level resource conflicts to identify preferable initial conditions and to evaluate the influence of stochasticity on the model; the similarity of outcomes within a threshold demonstrated the model's insensitivity to randomness. OAT's simplicity while attractive also exposes its limitations in ABM SA (Ligmann- Zielinska 2013). For one, the impactful and relevant values for each input parameter may be *a priori* unknown thus rendering any prioritization of parameters difficult and the search for key parametric drivers inefficient. Also, the marginal nature of the parameter search space surrounding the baseline obscures parameter interactions and severely shrinks the input hypercube with larger parameter sets. For example, with as few as 10 input parameters, OAT covers only 0.25% of the input space (for a geometric proof, see Saltelli and Annoni (2010)).

3.10 *Elementary effects* (EE) expands on OAT by relinquishing the strict baseline. That is, a change to an input parameter is maintained when examining a change to the next input rather than resuming the baseline value (as done in OAT). Passing over the parameter set is multiply repeated while randomly selecting the initial parameter settings. These perturbations in the entire parameter space classify EE as *global SA* (Saltelli et al. 2008). Originally proposed by Morris (1991) and improved by Campolongo et al. (2000), EE is suited for computationally expensive models having large input sets and can screen for non-influential parameters.

3.11 Global SA may also be performed through estimation of *standardized regression coefficients* (SRC), which in its basic form succinctly measures the main effects of the input parameters provided the relationships between the parameters and the outcomes are primarily linear. A standardized regression coefficient expresses the magnitude and significance of these relationships as well as the explained variance. More precisely, the square of the coefficient is the variance explained.

3.12 One glaring limitation of SRC is its ability handle spatial inputs (of spatial ABMs) unless a small set of scalars or indices can sufficiently serve as proxies for entire maps (Lilburne & Tarantola 2009). Also, SRC can expose lower-order effects but not complex interdependencies (Happe et al. 2006).

3.13 *Meta-modelling* (or emulation) can address the low-order limitations of SRC. A meta-model (emulator, a model of a model) is the surrogate representation of the more complex model (like ABM) created in order to reduce the computational time of the simulations necessary for SA. For example, Happe et al. 2006 collated model responses from a 2^k factorial design on a relatively small set of parameters and fitted a second-order regression. Meta-modelling can be computationally efficient and not necessarily require large amounts of data. For even higher order effects, meta-modelling methods such as Gaussian process emulators are required (Marrel et al. 2011).

3.14 *Variance-based* SA (VBSA) is considered the most prudent approach for evaluating model sensitivities as it does not assume linearity (Ligmann-Zielinska & Sun 2010; Fonoberova et al. 2013; Tang & Jia 2014). In VBSA, the total variance of a given output is decomposed and apportioned to the input parameters including their interactions (Saltelli et al. 2000; Lilburne & Tarantola 2009). Two indices per input (i) are drawn from the partial variances: a first-order (main effects) index S_i and a total effects index ST_i. S_i is the ratio of i's partial variance to the total variance. ST_i is the sum of all non-i indices ($\sum S_{-i}$) and captures interactions between i and the other inputs (Homma & Saltelli 1996). S_i alone is sufficient for decomposing additive models, so VBSA is unnecessary for models known to produce largely linear output as calculation of the index pairs is computationally expensive requiring large sample sizes (Ligmann-Zielinska & Sun 2010); for example, VBSA for k parameters requires $M(k+1)$ model runs where $M > 1000$. This computational load may be reduced through parameter (or factor) grouping (Ligmann-Zielinska 2013; Ligmann-Zielinska et al. 2014), parallelization (Tang & Jia 2014), or quasi-random sampling (Tarantola & Zeitz 2012). Situations in which inputs are exogenously correlated may result in non-unique VBSA (Mara & Tarantola 2012). While recent methods addressing these dependencies have been developed (Kucherenko et al. 2012; Mara & Tarantola 2012; Zuniga et al. 2013), they still require elaborate DOE coupled with a very large sample size and algorithmic complexity.

3.15 *Genetic algorithms* (GAs) may also be used for SA (Stonedahl & Wilensky 2010). Parameters are altered under the genetic paradigm of reproduction in which pairs of "fitter" parameter sets exchange subsets. The fitness (or objective) function may be tailored to expose model sensitivities to its parameters (as opposed to calibration). For example, Stonedahl and Wilensky (2010) allowed GAs to search through 12 parameters of the "Artificial Anasazi" ABM (Dean et al. 2000; Janssen 2009) in order to induce responses departing far from the empirical, historical values, while constraining the search to a limited range ($\pm$10% of their calibrated settings). See Figure 18 in Appendix D for a plot of the outlier results.

3.16 The reliance on mean and variance for distributional information in many of the practiced methods of SA is insufficient for more complex distributions. Future research should investigate moment-independent methods (Borgonovo 2007; Baucells & Borgonovo 2013).

Visualization in sensitivity analysis

3.17 Visualizations of the input parameter-output relationships are an integral part of SA. In *scatter-plots*, these relationships are directly and simply plotted potentially revealing dependencies (see Figure 5). We used the simple Schelling segregation model

(Schelling 1969) of red and green agents on a 100x100 grid implemented in Agent Analyst (http://resources.arcgis.com/en/help/agent-analyst/). The model contains four uniform parameters (lower and upper bounds in parentheses): number of agents (3000, 6000; discrete), tolerance to agents of different colour (0.2, 0.5), random seed (1, 10000; discrete), and percent of green agents (10, 50). We measured agent migration (total number of agent moves during model execution) for $N = 1280$ model runs.

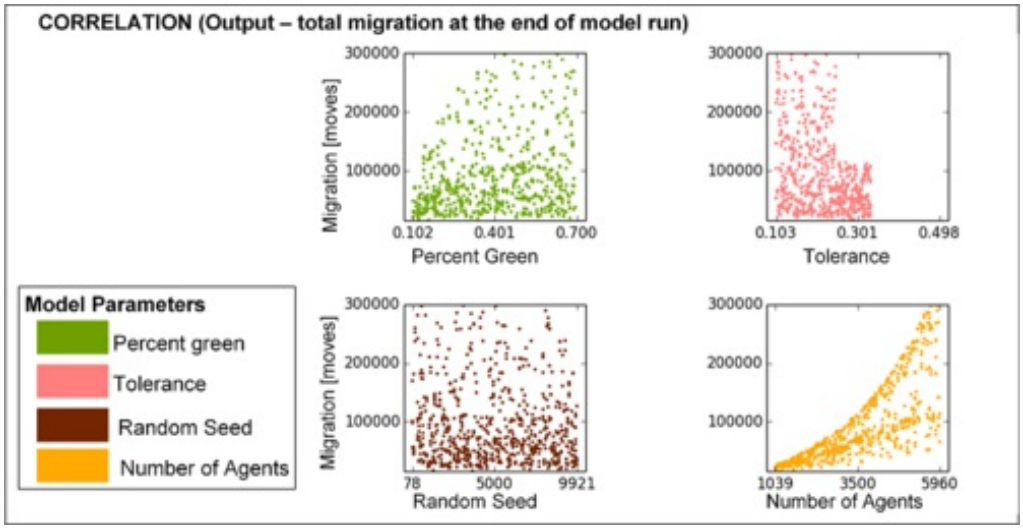


Figure 5. Sensitivity analysis with scatterplots. *Scatterplots of total migration versus the four model inputs at* $t = 100$; *note that number of agents has more influence on the variability of total agent migration than the other inputs.*

3.18 Typically, the y-axis and x-axis (for a two-dimensional scatterplot) express values for an output and an input parameter, respectively. Scatterplots are especially useful when the dependencies are structured, the output is a scalar, and the number of model parameters is limited allowing for an unencumbered enumeration of parameters and output combinations in separate scatterplots. More complex model behaviours require alternative visualization styles such as *pie charts* to display variance partitions (see Figure 6).

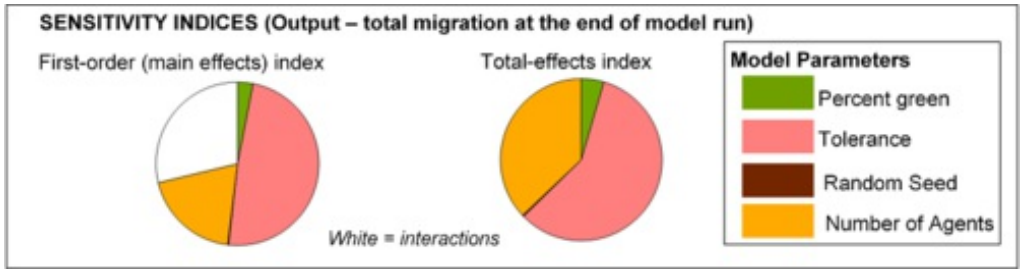


Figure 6. Sensitivity indices obtained from decomposition of migration variance at $t = 100$. *Note that almost 30% of migration variance is caused by interactions among inputs – mainly tolerance and number of agents.*

3.19 A snapshot of *variance decomposition* at the end of the model run (e.g., Figure 6) may be insufficient in assessing the importance of parameters and consequently their prioritization (Ligmann-Zielinska & Sun 2010). Thus, visualizing variance decomposition temporally will reveal parameter stability over the course of the model run (see Figure 7). Spatial outputs such as land use change maps may also receive similar treatment to reveal the extent of outcome uncertainty in regions (or clusters) due to specific parameters (Ligmann-Zielinska 2013).

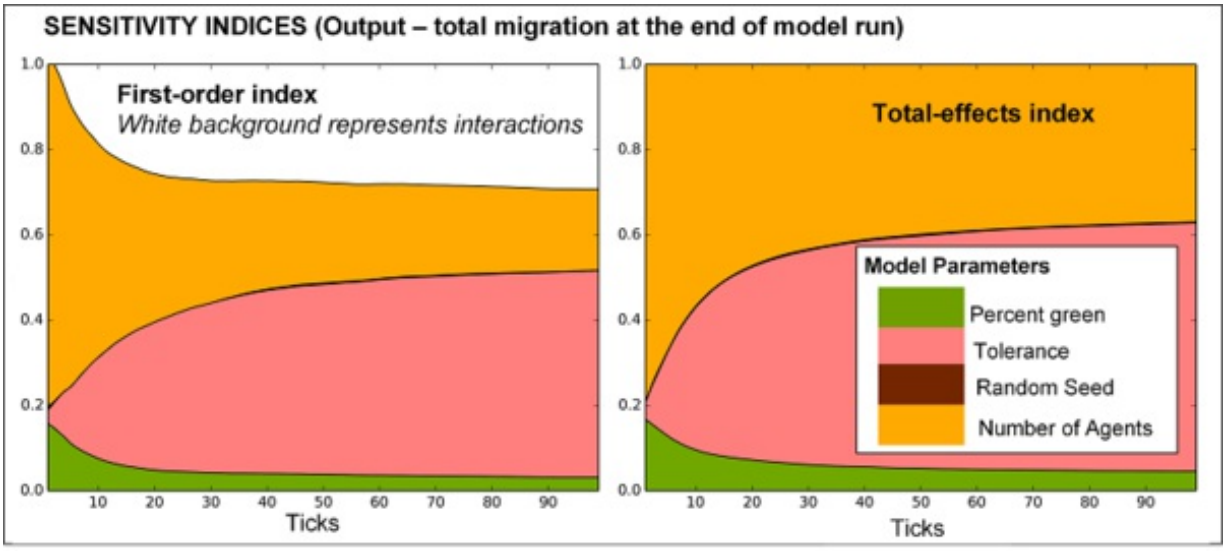


Figure 7. Time series of sensitivity indices obtained from decomposition of migration variance measured over time. *The example demonstrates that parameter sensitivities can considerably vary during simulation, with number of agents dominating the variance at* $t = 10$, *and tolerance dominating the variance at* $t = 100$.

3.20 SA for multiple outcome variables in an ABM incurs additional challenges due to differences in each parameter's impact on the outcomes (see Figure 4). This issue is of particular concern for model simplification and demands either one single, well-chosen outcome that is adequately representative of the model's behaviour or more conservatively, the difficult task of undergoing SA across the whole spectrum of outputs: scalars, time- and space-dependent measures.

Spatio-Temporal Dynamics

Temporal and spatial dimensions of ABM output data: challenges

4.1 As a stochastic process, an ABM generates (or is capable of generating) *time series* (TS) data. To a slightly lesser extent, ABMs also operate within topological boundaries often expressed as a spatial landscape, whether empirical (e.g., Parker et al. 2002; Bousquet & Le Page 2004; Heppenstall et al. 2012; Filatova 2014) or stylized (e.g., early use by Schelling 1969, 1978; Epstein & Axtell 1996). Similar to other ABM outcomes, both the TS and spatial data are borne out of complex endogenous dynamics over which the modeller exerts full control. Thus, it is rarely the case that the output data is produced by a single component of the model. Instead, most of ABM TS and spatial output recorded embody the long list of unique features that ABMs exhibit such as emergence rather than aggregation at the macro-level, interaction rather than reaction at the meso-level, and non-linearity rather than linearity of processes and decision-making at the micro-level. Spatial maps generated by ABMs may also capture eventual spatial externalities, path-dependencies, and temporal lag effects. These characteristics render the analysis of ABM outputs less appropriate for more traditional tools. These issues derive from the reasons ABM are used in the first place.[4] We consider this challenging nature of TS and spatial output analysis in the following sections.

Time: approaches and visualization techniques

Time series generated by ABMs (ABM TS) represent a myriad of temporal outcomes, such as evolving agent characteristics (e.g., sociodemographics, utility, opinions); agent behaviours/decisions (e.g., strategies, movements, transformations); or measures descriptive of the model state (e.g., agent population or subpopulation counts). All these are often presented as simple line graphs representing 1) outcomes of individual agents of special interest (Squazzoni & Boero 2002, Fig. 9) or 2) aggregated statistics (such as mean or median) over the entire agent population, subgroups, or an individual (with measurements over several runs) under varying levels of temporal granularity (e.g., a moving window covering several time points) (Izquierdo et al. 2008). Comparisons of multiple TS are often facilitated by the inclusion of confidence intervals (Raczynski 2004, Fig. 4) and occasionally performed against experimental/empirical (Richiardi et al. 2006; Boero et al. 2010, Fig. 1) or theoretical (Takahashi & Terano 2003, Fig. 4) outcomes or expectations (Angus & Hassani-Mahmooei 2015). TS comparisons have also been performed for calibration purposes (Richiardi et al. 2006).

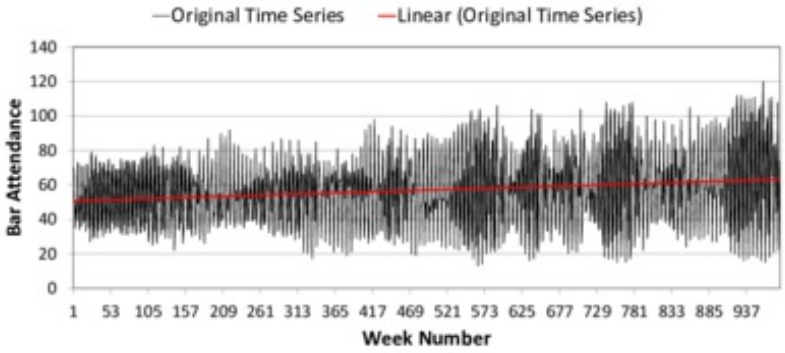
4.2 Despite the proliferation of ABMs, effective TS analytical techniques remain under-used (Grazzini & Richiardi 2015). Angus and Hassani-Mahmooei (2015) surveyed over 100 ABM publications in *JASSS* and found very few instances of additional (statistical) modelling of TS data. Only in agent-based financial market research does one find relevant TS statistical and econometric analysis (Yamada & Terano 2009; Chen et al. 2012; Neri 2012).

4.3 In this section, we discuss elements of TS analysis in the context of ABMs and present some basic and some compelling examples, while stopping short of expounding formal TS modelling such as auto-regressive models.

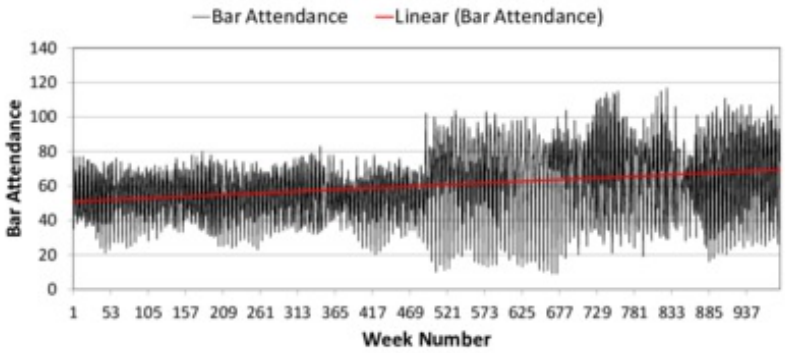
4.4 Among the techniques for analysing ABM TS, we consider *time series decomposition* to be one of the more useful methods. Decomposition entails partitioning a TS into four components: trend, cyclical, seasonal, and random components. The prominent *trend* is the most structured of these components and depicts the long-term linear or non-linear change in the TS data. The *seasonal* component exhibits regular periodicity due to some fixed external cycle such as seasons, months, weeks, or days of the year. Exogenous model events such as regular additions of a fixed count of agents to the agent pool are also considered seasonal. Cycles having irregular periodicity constitute the *cyclical* component. Finally, the residual or *random* component captures the unexplained variation remaining after the prior three components are filtered from the TS.

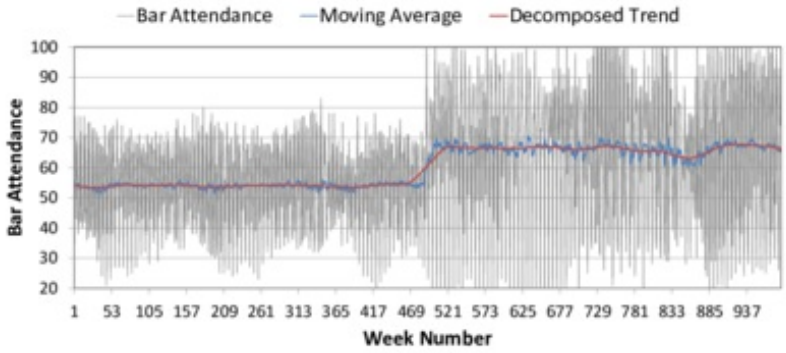
4.5 The spectrum of TS analysis techniques runs from the calculation of *moving averages* and *linear filtering* (see Figures 8a and 8b) to the more sophisticated *exponential smoothing* and *autoregressive modelling*. Furthermore, ABM relevant ergodicity tests may be applied to infer stationarity of statistical moments (e.g., mean, variance, skewness, kurtosis, etc.) hence equilibrium of those moments across a pool of simulation runs (Grazzini 2012).

4.6 For an example of ABM TS analysis, we examine the output of the well-known El-Farol "bar patron" game-theoretic ABM (Rand & Wilensky 2007). The initial conditions are: memory size = 5, number of strategies = 10, overcrowding threshold = 50. The number agents increases by 2% every 52 steps. Figure 8a presents the original data and its linear increasing trend (in red). Subtle structure in the TS is exposed when we plot a moving average along with its decomposed trend (obtained via exponential smoothing) (Figure 8b).



(a) Linear trend (b) Moving average





(a) Linear trend (b) Moving average

Figure 8. Time Series of Bar Attendance in El Farol ABM. *The black and grey series represent the original data; the red line is the linear fit (left) or decomposed trend (right); and the blue line is a moving average. The upper subfigures are labelled (a) and (b). The lower subfigures are (c) and (d).*

4.7 The model behaviour is augmented to include an arbitrary, one-time increase in population increase while the gradual increase is reduced to 0%. While the linear trend for the new results (Figure 8c) coarsely captures the population increase, the sudden change is made starkly visible using a moving average (plus decomposed trend) (Figure 8d).

4.8 Comparisons between TS drawn from distinct model parameterizations can be easily performed through direct (albeit naïve) visual comparison of the two series, plotting the differences, or calculating their *Euclidean distance*[5] or *cross correlation*. However, these comparison approaches are applied to exact temporal pairwise data and thus fail to account for the complexities of ABMs that may produce TS that are dissimilar only through interspersed lags. In addition to Richiardi's (2012) suggestions for robust TS comparison, we advocate the use of *dynamic time warping* (DTW) to address the above complication (Keogh & Ratanamahatana 2005). DTW is now extensively used in areas such as motion and speech recognition. Using a stylized pair of TS, Figure 9 depicts the effectiveness of DTW, which identifies comparable pairs of data occurring at differing time scales.

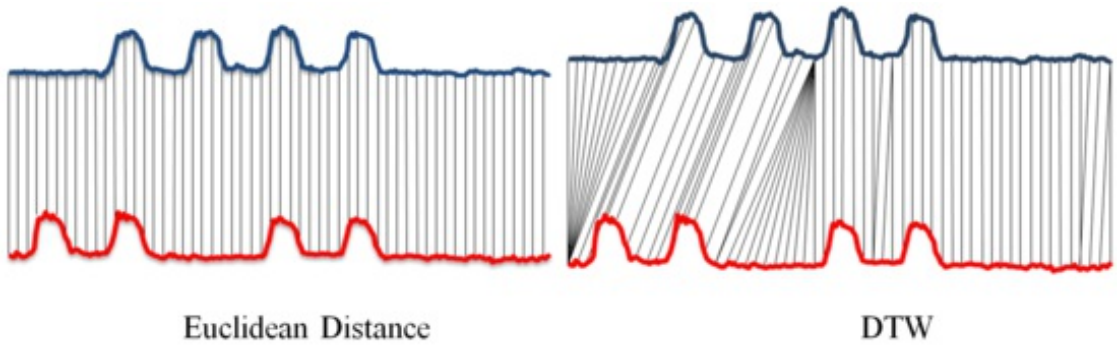


Figure 9. Comparing distance (similarity) measurement methods between Euclidean Distance (left) and DTW (right)

4.9 To further demonstrate DTW's effectiveness, we compare 40 distinct parameter settings in Epstein's ABM of civil violence (Epstein 2002; Wilensky 2004). The primary distinction is the initial cop density which ranges from 4.05 and 5.00 in increments of 0.05% and results in varied sizes of the population of quiet citizens, our outcome measure of interest here. We obtain 10 TS samples (i.e., model runs) under NetLogo each having a duration of 200 ticks/time points. In Figure 10, we present four individual runs in order to highlight the difficulty of direct visual comparison.

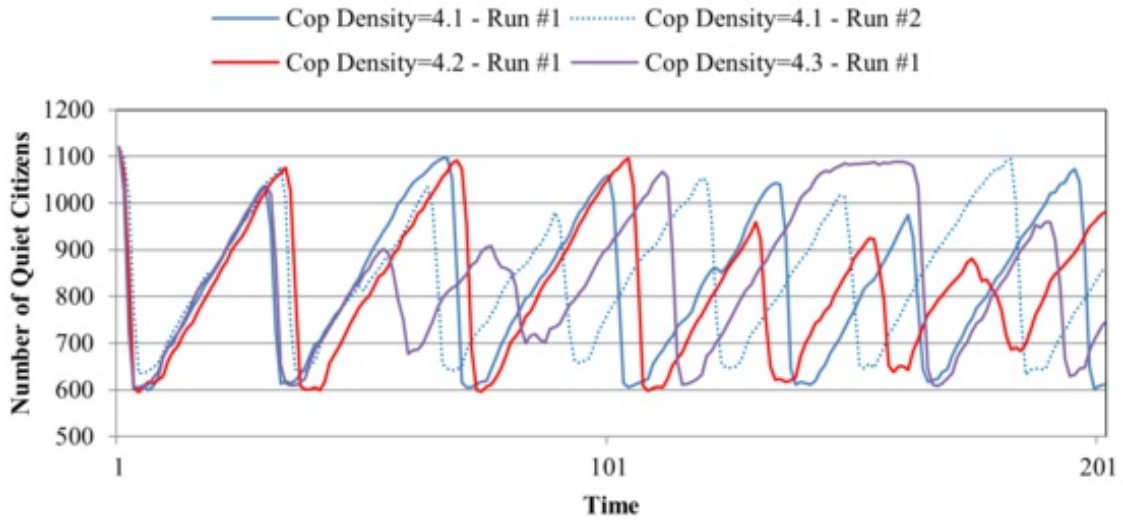


Figure 10. Comparing Time Series from Distinct Parameterizations of Quiet Citizens of Civil Violence ABM

4.10 While the outcomes are initially similar, they rapidly diverge sharing only the characteristic of the outcomes' exhibiting some fluctuation. The two runs under the same parameter setting (4.1%) naturally diverge due to distinct random sequences (from a RNG using distinct random seeds).

4.11 Comparisons of all pairs of the experimental conditions are presented in Figure 11. These comparisons are performed on normalized outcomes averaged over the suite of runs. The distance measurements in the left matrix are direct correlations and Euclidean distances in the right matrix. The cells in the upper triangle of each matrix correspond to direct comparison of the TS while those in the lower triangle indicates the measurements under DTW. The row and columns denote increasing cop densities.

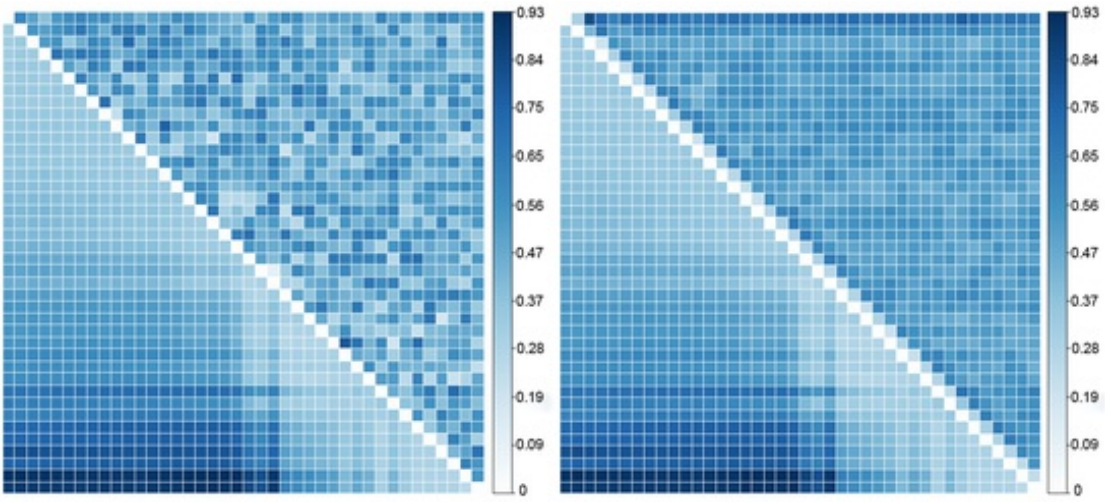


Figure 11. Comparing DTW against non-DTW for correlation and Euclidean distance

4.12 The figures illustrate the superiority of DTW in capturing TS differences under these measurements, over the direct use of exact temporal pairs. DTW clearly exposes greater similarity of the outcomes' TS when the experimental parameters (cop density) are also similar whereas the direct measurements do not. This relationship is largely monotonic as one would expect. Thus, DTW is appropriate for models for which the outcome TS's structure (specifically, both its seasonal and irregular periodicities) is greatly affected by the experimental conditions.

4.13 Finally, TS analysis provides a highly informative opportunity to precisely estimate the impact of changes in the input variables on the outputs of an ABM model. Techniques such as *panel data* (or *longitudinal*) analysis, which take into account both TS and cross sectional components of the data, can enable the agent-based modellers to uncover robust evidence on how model behaviours are associated with the changes in the variables of the agents and/or the model over time. Other prominent components of TS analysis (such as *forecasting*, *classification and clustering*, *impulse response function*, *structural break analysis*, *lag analysis*, and *segmentation*) may also be used along with estimation and auto-regressive methods in order to provide a better understanding of series generated by ABMs.

Processing spatial ABM output: approaches and visualization techniques

4.14 The spatial environment in ABMs vary from cellular grids (in which only inter-agent distance matter) to raster or vector representations of multiple layers of a rich GIS data. Locations in a spatial ABM may relate to output metrics at the individual or aggregated agent level (e.g., income, opinion, or a strategy) or other spatial qualities (e.g., land-use categories). It is challenging to seek patterns and to compare across experimental conditions in a search for a compelling narrative while screening through hundreds of maps produced by an ABM. Spatial ABM analysis is often informed by methods from geography and spatial statistics/econometrics. Here, we review some spatial metrics and visualization approaches for spatial analysis.

4.15 Quantitative indices such as the *Kappa index of agreement* (KIA or Cohen's κ) have been widely employed for cell-by-cell comparison of ABM outcomes on spatial maps (Manson 2005). More recent work suggest alternatives to the κ such as a *moving window* algorithm (Kuhnert et al. 2005) and expose its limitations (Pontius & Millones 2011). Pontius (2002) proposes more comprehensive methods and measures for tracking land use changes and comparing maps under multiple resolutions (from coarse to fine).

4.16 Various *spatial metrics* are often used to measure land-use change and detect spatial patterns such as fragmentation and sprawl (Parker & Meretsky 2004; Torrens 2006; Liu & Feng 2012; Sun et al. 2014). These metrics include mere counting of land-use categories, *landscape shape index*, *fractal dimension*, *edge density*, as well as *adjacency*, *contiguity*, and *centrality indexes*. *Moran's I* is another spatial autocorrelation statistic indicating the extent of dispersion or clustering (Wu 2002). Millington et al. (2008) used a *contagion index* along with basic patch count metrics to identify fragmentation. Griffith et al. (2010) used *Getis-Ord Gi* "hotspot" analysis* to identify statistically significant spatial clustering of high/low values while analysing the spatial patterns of hominids' nesting sites. Zinck and Grimm (2008) used spatial indices (*shape index*, *edge index*) and basic metrics (counts and areas of discrete "island" regions) to systematically compare empirical data to simulation results from the classic Drossel-

Schwabl forest fire cellular automata ABM. Software offering these metrics include C++ Windows-based 'FRAGSTATS' and the 'SDMTools' package (for the platform-independent R), the functionality of which may be augmented by Bio7 and ImageJ for image processing.

4.17 In another example, Sun et al. (2014, Table 6) reported basic statistics (i.e., mean and standard deviation) on nine spatial metrics estimated over multiple parameter settings for varying levels of land market representation in their urban ABM. The significance of mean differences (across conditions) were assessed with the *Wilcoxon signed rank test*. Means of the metrics were jointly visualized across all parameter settings in a line graph style called "comprehensive plotting" (Sun et al. 2014, Figures 5–8), which then allows for identification of conditions producing outlying behaviour facilitating visual sensitivity analysis.

4.18 Obviously, statistical models such as regressions and ANOVAs may be employed to relate model parameters and outcomes to spatial outcomes (e.g., Filatova et al. 2011). However, dependencies among spatially distributed variables require special treatment in the form of a weighted matrix incorporated into a *spatial regression model* as a predictor or as part of the error term. Locales may be disambiguated further in statistical prediction through *geographically weighted regression* (GWR). These methods also fall under the auspices of spatial econometrics.

Reporting and visualizing ABM results over time and space

4.19 Typically, spatial ABM output is rendered as two-dimensional maps. A collection of these can highlight model dynamism/progression or allow for comparison of metrics and experimental conditions (Parry & Bithell 2012, Figure 14.11) or expose key, informative trajectories (e.g., Barros 2012, Figure 28.3). 3D views are also used to portray outputs particularly in evacuation and commuting (Patel & Hudson-Smith 2012). Often, visual inspection of the data offers face validation and high-level inference. For example, a *spatial overlay* is commonly used to analyse raster outputs and evaluate the spatial distribution of multiple model behaviours and outcomes.

4.20 The spatial distribution of outcomes is subject to the stochastic and path dependent nature of ABMs and often demand aggregation for effective presentation of model behaviour (Brown et al. 2005). Naturally, a mean with a confidence interval for an outcome in each spatial location can be sufficient for reporting a set of maps (over time or across experimental conditions) (e.g., Tamene et al. 2014). Alternatively, a *frequency map* for a single parameter setting reveals each location's state transition probabilities (as a proportion of total simulation runs) (Brown et al. 2005). These transitions may easily be portrayed as a *colour-gradient* map (e.g., Magliocca 2012). Plantinga and Lewis (2014) warn against constructing deterministic transition rules out of these probabilities. Brown et al. (2005) also suggest distinguishing areas of non-transition (or invariant regions) from variant regions; the method for identifying these areas is called the *variant-invariant method*.

4.21 Judicious selection of a temporal sequence of maps can reveal model dynamics. Software such as a "map comparison kit" (RIKS BV 2010) can perform automated tests to identify the extent to which two raster maps are different. Pontius et al. (2008) extends the comparison exercise to include three maps while considering pixel error and location error. Comparisons include all pairs of simulation outputs at times 1 and 2, a "true", reference map at time 2, and all three maps jointly.

4.22 While showcasing a map as an output of an ABM is always appealing, supplementing it with summary statistics of spatial patterns allows for deeper understanding of experimental effects and consequently the model's behaviour. In addition to the spatial metrics discussed in 4.3, quantities of land use and conversions may be reported as histograms across different scenarios and land-use types over time (e.g., Figure 4 in Villamor et al. (2014)).

4.23 Color-gradients in landscape visualizations can be used to represent temporal changes in a metric of interest. Filatova (2014) employs these *spatio-temporal change gradients* to present land price changes (due to market trades in an ABM focusing on coastal properties) between two points in time in an empirical landscape (Figure 12).

Figure 12. Changes in property prices over time

4.24 The blue and red gradients correspond to the valence of the change (i.e., falling and rising prices, respectively); their darkness or

intensity indicate level of change. Such visualizations may offer easy identification of clusters and boundaries.

4.25 Another obvious way to depict the differences in spatially distributed ABM output data is to visualize in 3D plots. The 3rd dimension clearly permits the inclusion of additional information such as time or one of agents' inner attributes. For example, Huang et al. (2013) employed 3D colored bar plots (Figure 13) in which the 2D layout corresponds to physical location.

4.26 Such 3D visualizations offer insights into the ABM's dynamics or highlight vital structural differences across experiments. For example, Dearden and Wilson (2012) use a 3D surface to plot the macro metrics of interest of their retail ABM as a function of different values of the two most critical parameters affecting agents' choices. 3D surfaces over different parameters spaces can also be compared with each other, as demonstrated by Dearden and Wilson in their comparisons of activity within consumer and retailer agent classes.

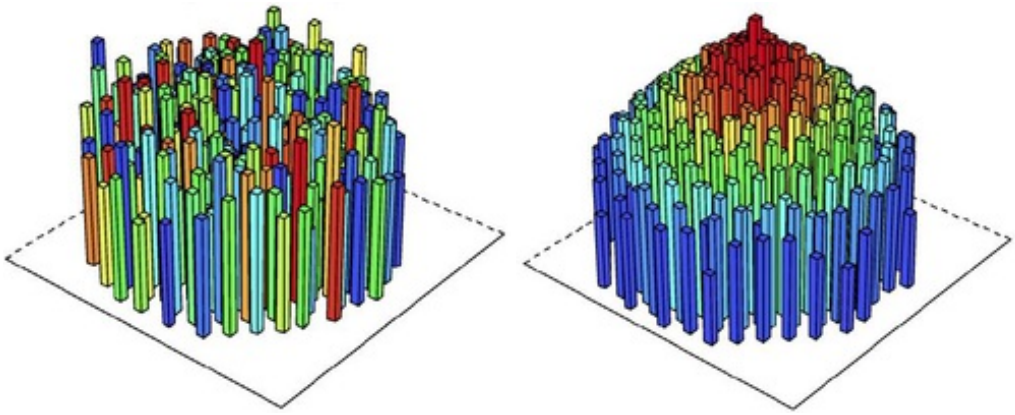


Figure 13. Price of land and sequence of transactions under various market conditions when agents have heterogeneous preferences for location. *Left: Allocation of land on this market is only preference driven. Right: Land allocation happens through competitive bidding. The higher the bar, the higher the land price. colours denote the time when land was converted into urban use.* Source: Huang et al. (2013)

4.27 In this example, the color adds a fourth dimension (time of an event) to the conveyed information. Furthermore, functional shapes are more easily discernible in 3D; in this case, the upper section of Figure 13b might be fitted to a paraboloid or a similar solid of revolution.

4.28 Another efficient use of 3D visualization for ABMs with geo-spatial elements is shown in Figure 14. Malleson's model of burglary in the context of urban renewal/regeneration comprises agents who travel to commit crime in an urban landscape (Malleson et al. 2013).

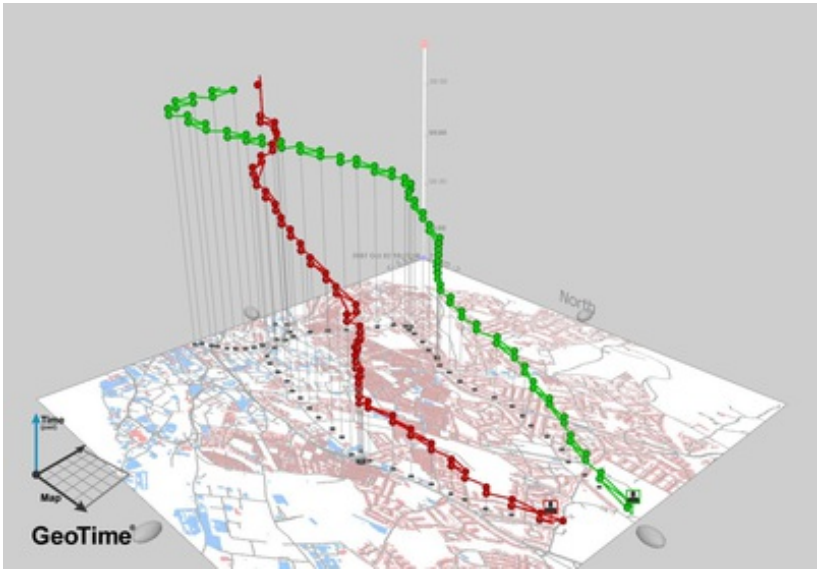


Figure 14. Spatio-temporal Trajectories of Burglars. *Source: Nicolas Malleson. http://nickmalleson.co.uk/research*

4.29 The colored, segmented lines in the figure when overlaid onto the *2D city map* depict the trajectories of burglar agents seeking targets while the *z-axis denotes the temporal dimension* to their journey. This joint portrayal of time and space succinctly communicates important features such as key locations of activity for the agents (i.e., where lines appear vertical) as well as the origin of the agent and its destination, in this case a presumably "safe" location.

4.30 Finally, given the dynamic nature of ABMs, their spatial and temporal outputs are appropriate for dynamic presentation modalities. Interactive 3D visualizations offer the ability to examine the data from alternative perspectives. Increasingly, *video* (or animation) has been used to capture ABM behaviour as a means to communicate ABM output to both practitioners as well as the

broader lay-audience.[6] Model behaviour may also be captured as *animated GIF files*, the small sizes of which facilitate their use in presentations and web pages (Lee & Carley 2004; Lee 2004).

Discussion and conclusions

5.1 While ABM as a technique offers many exciting opportunities to open research frontiers across a range of disciplines, there are a number of issues that requires rigorous attention when dealing with ABM output data. This paper highlights the outstanding complexities in the ABM output data analysis and consolidates currently-used techniques to tackle these challenges. In particular, we group them into 3 themes: (i) *Statistical issues related to defining the number of appropriate runs and hypothesis testing*, (ii) *Solution space exploration and sensitivity analysis*, and (iii) *Processing ABM output data over time and space*. We also briefly discuss *stakeholder involvement in ABM research* (iv) below.

5.2 Statistical issues related to defining a number of runs and hypothesis testing: For analysing ABMs, the calculation of statistics from model outcomes across multiple simulation runs is required. However, the statistical methods are challenged by both a plethora of ABM output data for which traditional statistical tests will expose minute effects and complex ABMs for which runs are costly. In the former scenario, statistical methods need to be tempered (e.g., a more critical p-value) or an acceptable ceiling on the number samples (or runs) should be enforced. For the latter case, a predetermination of test sensitivity (e.g., effect size) must be made before calculating a minimum number of runs. However, the stability of outcome variance needs to be secured, and we demonstrate and review approaches for estimating the point at which this is achieved. We also reveal that the traditional approach to determining minimum sample size is sensitive to the shape of the distribution and we suggest empirical estimation of the power level or use of the more conservative Wilcoxon rank sum test. Another challenge is the analysis of many influencing variables. The analysis of complex interdependencies within a simulation model can be addressed by systematic design of experiment principles, and univariate analysis may support the analysis by pre-defining parameter ranges. Overall, ABM researchers should be aware of the statistical pitfalls in the analysis of simulation models and of the methods described to address these challenges.

5.3 Solution space exploration and sensitivity analysis: An ABM cannot be properly understood without exploring the range of behaviours exhibited under different parameter settings and the variation of model output measures stemming from both random and parametric variation. Accordingly, it is important for ABM analysts and researchers to be familiar with the range of methods and tools at their disposal for exploring the solution space of a model, and for determining how sensitive model outputs are to different input variables. ABMs pose particular challenges for SA, due to the nonlinearity of interactions, the non-normality of output distributions, and the strength of higher-order effects and variable interdependence. While some model analyses may find success using simple/classic SA techniques, practitioners would do well to learn about some of the newer and more sophisticated approaches that have been (and are being) developed in an effort to better serve the ABM community.

5.4 Processing ABM output data over time and space: While every ABM has the potential to produce high resolution panel data on aggregated and agent-level metrics over long time periods, the standard time series techniques are rarely applied. We argue that the use of time series techniques such as decomposition and moving averages analysis not only improve the scientific value of ABM results but also help gaining valuable insights – e.g., the emergence of the two regimes in the data over time – that are likely to be omitted otherwise. The use of Euclidean distance similarity measurement and dynamic time warping offers high utility especially when temporally varying outputs need to be compared between experiments or in a sensitivity analysis exercise. When dealing with spatial data analysis, ABM researchers actively use methods developed in geography such as spatial indexes, map comparison techniques, series of 2D or 3D maps, 2D histograms, and videos. In addition, ABM-specific methods are being actively proposed – such as 3D histograms reflecting temporal changes over a spatial landscape, spatio-temporal output variable change gradients, as well as overlaying temporal ABM dynamics over a 2D map.

5.5 Communicating ABM results to stakeholders: The utility and effectiveness of many ABMs and their outputs are often judged by the model's consumers: the user, the stakeholder, or decision-maker. Thus, a qualitative understanding of the model is essential as model acceptance and adoption depend strongly on subjective, qualitative considerations (Bennett et al. 2013).

5.6 The clarity and transparency of ABM mechanisms facilitate stakeholder involvement in the modelling process. This participatory modelling is a powerful strategy to facilitate decision-making, management, and consensus building (Voinov & Bousquet 2010). In contrast to other techniques such as System Dynamics (SD), Computational General Equilibrium, or Integrated Assessment Modelling, ABM rules are explicit, directly embedded in the model, and do not necessarily have to be aggregated or proxied by obscure equations. Thus, ABMs have been historically at the forefront of participatory modelling. Communicative graphical user interfaces (GUIs) in platforms such as NetLogo and Cormas have also contributed to the clarity in presentation and ease of interpretation (as they have done for SD's Stella or Vensim). A clone of participatory modelling with ABMs conceived by French modellers became known as *companion modelling* (Bousquet et al. 1999; Barreteau et al. 2003; Étienne 2014) and is applied globally particularly in developing nations (Becu et al. 2003; Campo et al. 2010; Worrapimphong et al. 2010). As the focus is on the model as a process rather than a product (Voinov & Bousquet 2010), co-learning between stakeholders and modellers results in expedient cycles of modelling, output presentation and discussion, and subsequent amendment of the model.

5.7 Moss (2008) notes that evidence should precede theory, whenever modelling becomes embedded in a stakeholder process. Thus, interpretation of model outputs requires more than mere quantitative evaluation and interpretation, and the necessary task of weighing model outputs against values and perceptions of both stakeholders and modellers alike continues to challenge us

(Voinov et al. 2014).

5.8 Directions for future research: Most of the challenges and techniques considered in this paper are quite computationally intensive. Yet, the fact that an analysis of ABM output data often requires more time and attention than the design and coding of an ABM itself is still largely underestimated especially by amateurs in the ABM field. Thus, user-friendly software products that support design of experiments (e.g., the AlgDesign package in R (Wheeler 2011)),[7] parameter space exploration, sensitivity analysis, temporal and spatial data exploration are in high demand. For example, the MEME software is one step toward this goal and is a valuable tools for ABM researchers. ABMs would ideally support real world decision-making, hence efficient, user-friendly ABM platforms, supporting data analysis and visualization, would reinforce use of ABM in participatory modelling. Moreover, insights into advanced statistical techniques could assist in resolving some of the statistical issues discussed in Section 2.

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Notes

[1]This paper was inspired by a workshop at the 2014 iEMSs conference: the G2 workshop "Analyzing and Synthesizing Results from Complex Socio-ecosystem Models with High-dimensional Input, Parameter, and Output Spaces". During that workshop, several key issues facing today's simulation modellers were identified and discussed. The ones deemed to be more exigent have become the focus of this paper.

[2]The normal or Gaussian distribution also known as the "bell-curve" is the most easily recognized empirical distribution containing a single mode and often captures many naturally observed outcomes. The uniform distribution is a flat, artificial distribution and can be considered to serve as the control distribution among this set. The exponential is often used to model failure rates and is amodal and skewed. The Poisson expresses the probability of a given number events occurring within a known interval. The χ^2 (chi-squared) is typically employed in statistical tests as well as the Student's *t* distribution. We include these two as they are readily recognizable by many practitioners of applied statistics.

[3]The effect size calculation we employ is Cohen's d (Cohen 1988): $d = \frac{\mu_1 - \mu_2}{s_{\text{pooled}}}$.

[4]LeBaron et al. (1999, p. 1512), for example, note that their artificial stock market has time series capturing phenomena observed in real markets, including weak forecastability and volatility persistence.

[5]

$$\text{Euclidean distance} = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$$

where n is the number of data points in each vector.

[6]For examples, we cite Epstein & Axtell (1996) and the corresponding video: https://www.youtube.com/watch?v=SAXWoRcT4NM and Helbing et al. (2005) and the corresponding video: https://www.youtube.com/watch?v=yW33pPius8E.

[7]Further options in R for DOE may be found at http://cran.r-project.org/web/views/ExperimentalDesign.html.

Appendix A: Minimum Sample Size for Distributions

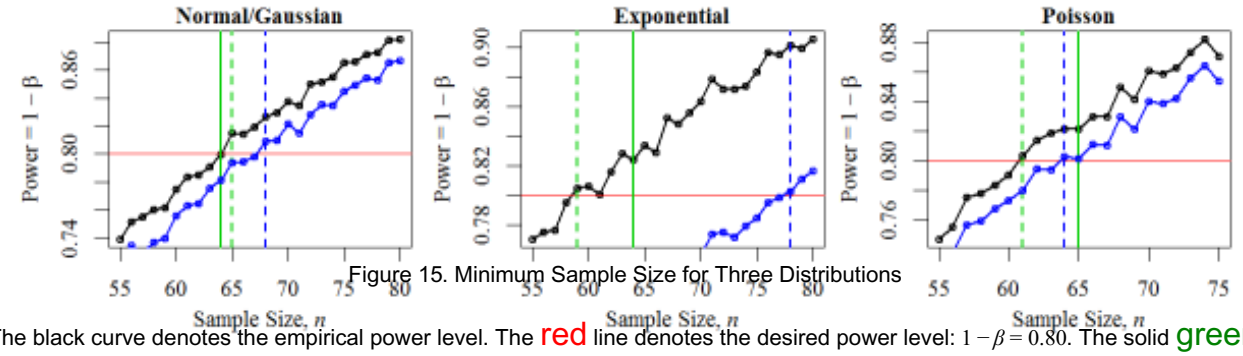

Figure 15. Minimum Sample Size for Three Distributions

The black curve denotes the empirical power level. The red line denotes the desired power level: $1-\beta = 0.80$. The solid green vertical line denotes the minimum sample size derived from the power calculation while the dotted green line shows the empirically-derived size. The blue curve and line denote the power and minimum size according to the two sample Mann-Whitney-Wilcoxon test.

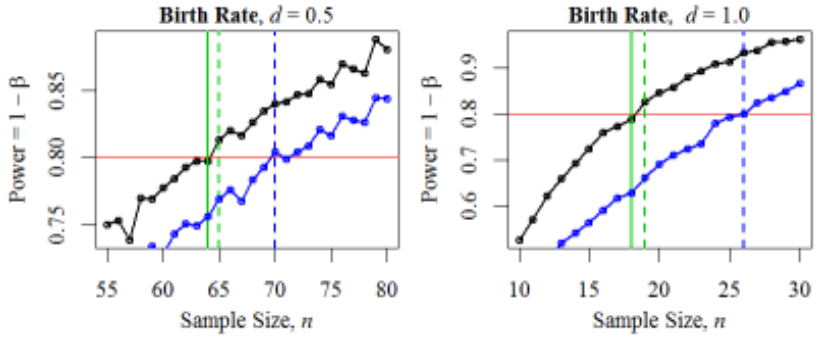

Figure 16. Minimum Sample Sizes for Birth Rate ABM

The red line denotes the desired power level: $1-\beta = 0.80$. The solid green vertical line denotes the minimum sample size from the power calculation; the dotted green line shows the empirically- derived size; and the blue curve and vertical line denote the power and minimum sample size according to the Mann-Whitney-Wilcoxon test.

Appendix B: Issues of Hypothesis Testing

There exists an ongoing debate over the emphasis researchers should place on significance tests. A large sample size can easily classify a minute difference as being significant. Thus, many (in the ABM field and outside) argue for greater attention paid towards the effect size itself (whether it is *Cohen's d* or a *standardized regression coefficient*) as the benchmark for a "significant" finding (Coe 2002; Ziliak & McCloskey 2008, 2009; Sullivan & Feinn 2012; White et al. 2013; Troitzsch 2014). In fact, recently the journal of *Basic and Applied Social Psychology* has implemented policy to remove p-values from their publications. Alternatively, researchers may turn to methods and measures that penalize (or minimize the impact of) large samples sizes. Rouder et al. (2009) demonstrate the effectiveness of such penalties in measures such as the *Bayesian information criterion* and the *JSZ Bayes factor*. Cameron and Trivedi (2005, p.279) suggest using $\sqrt{\log n}$ as a more stringent, critical *t*-statistic. An earlier suggestion by Good (1982, 1984, 1992) entails *adjusting the critical p-value using a sample size of* $n = 100$ as a reference point rather than leaving it fixed (e.g., $p < 0.05$) for all sample sizes. Furthermore, the estimated minimum sample size may be reduced through *variance reduction by control variates* which are outcomes having known mean and variance and are sufficiently correlated with other outcomes of interest for which the mean and variance are unknown. This technique is discussed in the context of simulation models by Law and Kelton (2007). Finally, sample size determination for large simulations which are costly to run (i.e., demanding heavy computing resources and incurring long execution times) may be addressed through bootstrapping of a smaller set of outcomes for estimating their variance (Lee & Carley 2013).

Appendix C: Multi-Modal ABM Output of Birth Rate ABM

Multi-modality in the output may indicate separate attractors in the phase space bridged by tipping points. For example, the output distribution (a subpopulation) of a simple, population genetics ABM (Wilensky 1997, 1999) under a single parameter setting exhibits clear bimodality (Figure 17). The carrying capacity was set to 200; the fertility rate for both red and blue populations was 2.0; and 10000 runs of 300 steps were performed.

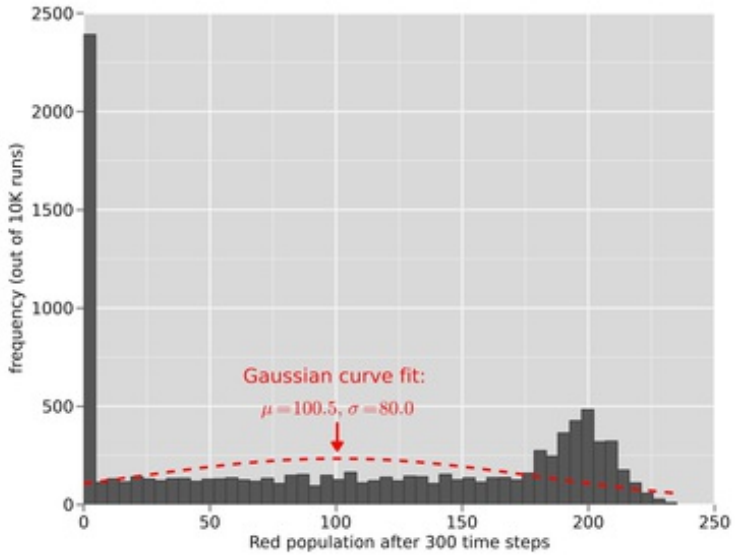

Figure 17. Birth Rate ABM Output Distribution. *Histogram of the "red" population after 300 times steps, fitted to a Gaussian curve (from the NetLogo Simple Birth Rates Model (Wilensky 1997))*

Interpreting the mean red agent population of 100.5 (with a large degree of error) as being singularly and truly descriptive of the stochastic process would be grossly inaccurate and overlook the salient bifurcation in which the red agent population tends to either diminish to extinction (0) or dominate (around 200). This example illustrates how ABM stochasticity may produce non-normally distributed output that cannot be sensibly described by merely its mean and variance.

Appendix D: Anasazi Model Outliers

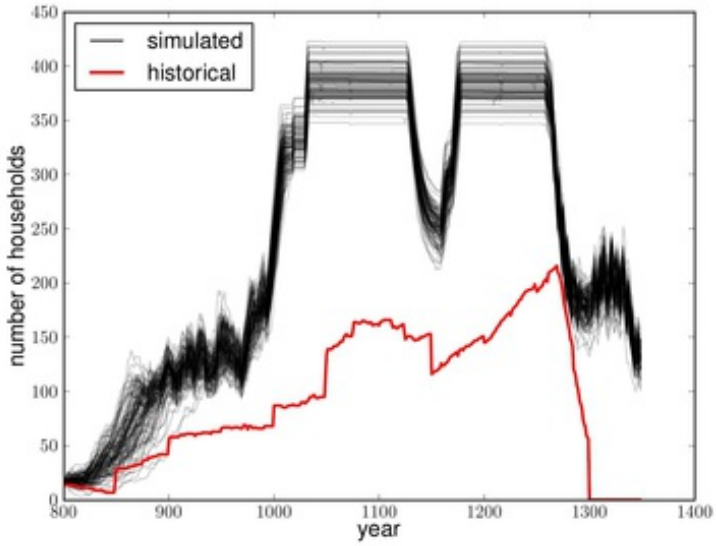

Figure 18. Sensitivity analysis example. *Source: Stonedahl and Wilensky (2010)*

The red line denotes the historical data and the black lines represent outcomes from 100 simulated runs parameterized (via a GA search) to produce output time-series that maximally differ from the historical data.

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