

# Easing Parameter Sensitivity Analysis of Netlogo Simulations using SPARTAN

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## Abstract

In attempts to further understand complex systems at an individual level, the application of agent-based modeling is becoming prevalent across a range of academic disciplines. With the advantages of being multi-platform, requiring little programming experience, and supported by a large number of freely available case study examples, Netlogo has become a popular choice as the software tool to apply in the construction of agent-based models. To utilize the constructed model as an informative or predictive tool, statistical analyses can be performed to reveal the influence that a parameter has on simulation behavior, offering an insight into the system under study. Here we demonstrate the integration of Netlogo's parameter sweep function, Behavior Space, with an extended version of SPARTAN, our previously published open source statistical package for performing local and global sensitivity analyses. With the addition of SPARTAN, the researcher can automatically create Netlogo experiment files for both local (individual parameter) and global (latin-hypercube and Fourier frequency) analyses, run these experiments in Netlogo, and receive detailed statistical information on the influence a parameter has on simulation response: vital information for translating a simulation result to a hypothesis grounded in the system being studied. To ensure our example work is reproducible, we demonstrate use of SPARTAN using the Virus transmission and perpetuation model available in the Netlogo model library.

## Introduction

As the application of agent-based modeling has become adopted across a range of academic disciplines, including biological, sociological, and economic, much focus has been placed on the release of software tools to aid the generation of a simulation of a system under study. One such popular toolkit is Netlogo (Wilensky, 1999), a freely available, multi-platform toolkit that aims to ease the construction of multi-agent systems. Simulations have been generated for a wide range of applications, recent examples being to inform government energy policy (Lee et al., 2014), to simulate trout demographics in a brook system (Frank and Baret, 2014), and emergency procedure planning for building evacuation (Wagner and Agrawal, 2014).

Previously we have demonstrated that our bespoke agent-based model, not generated in Netlogo, can create emer-

gent cell behavior that is statistically similar to that observed experimentally (Patel et al., 2012; Alden et al., 2012), providing a tool through which hypotheses concerning the formation of lymphoid tissue formation can be developed and tested. In the course of understanding the relationship between our simulation and the biological system that it represents, we developed SPARTAN (Simulation Parameter Analysis R Toolkit Application) (Alden et al., 2013), a package of statistical techniques specifically designed to aid researchers in translating a simulation result to an hypothesis grounded in the real-world domain. SPARTAN is open source and freely available from either the R package repository (CRAN) or from [www.ycil.org.uk/software/spartan](http://www.ycil.org.uk/software/spartan). To the best of our knowledge this was the first time a comprehensive package had been made available that could be applied to agent-based as well as traditional ordinary and partial differential equation models. Alongside the release of the package, we demonstrated the potential the included parameter sensitivity analysis techniques have in revealing the influence particular simulated pathways and components could have on the biological system.

The initial demonstration of SPARTAN utilized our lymphoid tissue simulator, a bespoke agent-based software tool created in Java with the aid of the MASON Simulation toolkit (Luke, 2005). In this case, we utilized SPARTAN in the creation of parameter value sets, performed simulation runs under the generated parameter conditions, and used the relevant SPARTAN technique to analyze the results. With this approach proving fruitful in understanding the behavior of our simulator, we have recently extended SPARTAN to enable researchers who use Netlogo to perform both local and global sensitivity analyses of their agent-based models. Although Netlogo is equipped with the Behavior Space feature, which allows the researcher to perform a sweep of potential parameter values, the researcher is required to develop routines for analyzing the resultant simulation responses. Recent work has been undertaken to link Netlogo with statistical environments such as R (Thiele et al., 2012), but does not provide statistical algorithms to fully understand the relationship between a simulation and the

system it represents. Here we demonstrate how combining Netlogo with SPARTAN provides the researcher with the tools to perform both parameter sampling and the analysis of the resultant simulation data, for three sensitivity analysis techniques. Firstly we describe the model that we have chosen to use, a virus transmission and perpetuation model (Wilensky, 1998) that is available in the Netlogo Model Library. We then briefly discuss the three sensitivity analysis techniques that are included within the SPARTAN package (one local analysis, two global analyses), before describing the result of each analysis for simulation responses generated from the Netlogo model. This paper is supported by a full tutorial demonstrating how each technique can be applied to the virus transmission model, available both within the SPARTAN package and accompanying website ([www.ycil.org.uk/software/spartan](http://www.ycil.org.uk/software/spartan)).

### The Case Study: Virus Transmission and Perpetuation

To aid the adoption of SPARTAN by researchers utilizing Netlogo, we believed that it was important the demonstration we include here and in the tutorial can be easily replicated. Thus we utilize a simulator that is freely available in the Netlogo Model Library, with a number of modifications that we describe here.

The Virus model (Wilensky, 1998) simulates a human population, to suggest how a virus transmits and is perpetuated amongst that population based on factors suggested by ecological biologists (Yorke et al., 1979). A full description of the composition of the model is included with the simulation. For our interests, there are four parameters that can be set by the researcher utilizing the model: the number of people in the population (*people*), the ease at which the virus spreads (*infectiousness*), the probability a person recovers from the virus (*chance-of-recover*), and the duration in weeks after which the person either recovers or dies (*duration*). Here we will demonstrate the use of SPARTAN in determining how both robust these parameters are to perturbation and the relative influence of each parameter on simulation response.

Such judgments are dependent on an analysis of how the chosen parameter values impact a set of simulation responses at a specified simulation time-point. As the current version of the virus model has no defined end point, we have modified the simulator such that the simulation runs for a 100 year period. With the simulator specifying that a persons lifespan is 27 years if they are not killed by the virus, modeling an 100-year time-period is sufficient for our needs. In terms of output response, the simulator provides the percentages of the population that are infected and immune. As we want our analysis to be representative of the entire period rather than a snapshot of the population, we introduced four additional output measures: the number of people who have died through not recovering from the in-

fection (*death-thru-sickness*), the number who died but were immune (*death-but-immune*), the number who died through old age and never caught the infection (*death-old-age*), and the number of people who died while infected but during the time period allowed for recovery (*death-old-and-sick*). As we are utilizing statistical tests to determine how alterations to the four input parameters described in the previous paragraph affect these responses, which are all numbers of people, we exclude the *people* parameter from the analysis, and run all our experiments with an initial population of 150 people, leaving three input parameters of interest. Additionally, to run the eFAST analysis that will be described later, an additional global parameter is added (*'dummy'*), that has no impact on simulation response. The reasoning for this becomes clear in later sections of this paper.

To ease the reproduction of results in the latter sections of this paper, we have made the modified version of the model available from the SPARTAN website ([www.ycil.org.uk/software/spartan](http://www.ycil.org.uk/software/spartan))

### Overview of Sensitivity Analysis Techniques in SPARTAN

In this section, we note the three parameter sensitivity analysis techniques available within the SPARTAN package. As we have previously described the full detail of the implementation of each technique, we cover each only briefly, and would direct you to our previously published work for the complete description (Alden et al., 2013; Read et al., 2012). The section that follows this details the application of each technique to the Netlogo Virus model.

#### Technique 1: Parameter Robustness

The parameter robustness technique examines the implications of any uncertainty or parameter estimation on simulator response. This highlights any parameters for which the simulation is sensitive to value perturbation, potentially suggesting that caution should be applied as a response may be an artifact of parameterization and not representative of the system that has been captured (Helton, 2008).

Parameter robustness is determined by perturbing each parameter independently of all others, which remain at their baseline value. Simulation responses under the perturbed conditions are compared with simulation response for baseline parameter values using the Vargha-Delaney A-Test (Vargha and Delaney, 2000), an effect-magnitude test used to determine if there is a statistically significant difference between simulation responses under differing conditions. For each parameter, SPARTAN produces two plots: the first detailing the A-Test response for each value it has been assigned, easing identification of parameter values that may cause a significant change in behavior, and a second showing the distribution of simulation responses for each parameter value.

## Technique 2: Global Sensitivity Analysis using Latin-Hypercube Sampling

Whereas robustness analysis perturbs each parameter individually, both this and the next technique seek to identify any compound effects that are revealed when the values of all parameters of interest are perturbed simultaneously. This global sensitivity analysis exposes cases where the effect one parameter has on the simulation response is dependent on the value of another, and can indicate the parameters having greatest influence on simulation response. Where a simulation bears a strong relationship to the real system being modeled, such an analysis has the potential to offer significant insight into the system under study.

This technique selects a number of simulation parameter value sets using latin-hypercube (LHC) sampling. LHC selects a value for each parameter from a specified range, while ensuring efficient coverage of the parameter space and minimizing correlations between chosen value sets (Read et al., 2012; Marino et al., 2008; Saltelli et al., 2000). Simulations are then performed for each generated set of parameter values. A plot is produced by SPARTAN for each parameter-simulation response pairing, revealing correlations between parameter value and simulation response. For reporting purposes, this correlation is also quantified through calculation of the Partial Rank Correlation Coefficient (PRCC), which is reported in the plot header.

## Technique 3: Global Sensitivity Analysis using Extended Fourier Amplitude Sampling Test

Whereas Technique 2 identifies compound effects using a sampling-based method (the hypercube), the extended Fourier amplitude sampling test (eFAST) (Saltelli, 2004; Saltelli and Bollardo, 1998) has been included in SPARTAN to offer an alternative: global analysis by variance decomposition. Variance in simulation output is partitioned between the parameters of interest, providing a statistical measure that reveals the proportion of variance that can be explained by the perturbation of each parameter. Such a measure is a key indicator that a parameter has a highly influential effect on simulation response.

Of the three techniques we are describing here, this is by far the most complex, and the reader is directed to our previously published work for the full detail of the algorithm (Alden et al., 2013). As a brief overview, each parameter is taken in turn as that of interest. These are accompanied by an extra parameter, the 'dummy', which has an arbitrary range of values and no impact on simulation response. Sinusoidal curves of a particular frequency are created in the parameter space, with the parameter of interest assigned a frequency that is significantly different to the remaining parameters in the analysis. From each curve, a specified number of values are chosen, in turn creating a number of parameter value sets for that parameter of interest (see Marino et al., 2008 for an illustration of this approach). A phase shift is employed that

shifts the frequency slightly, and the sampling repeated to mitigate the potential for identical value sets to be selected. This leads to the selection of a number of parameter value sets for each parameter, for each phase shift.

Simulations are executed for each of the parameter value sets generated in this process. The responses are analyzed by SPARTAN, taking into account the frequencies that were used in the generation of the parameter set. Fourier analysis is used to partition variance in simulation response between the parameters, and two statistical measures produced for each parameter: the fraction of output variance that can be explained by that parameter ( $S_i$ ) and the output variance caused by higher-order non-linear affects between the parameter and the others being studied ( $ST_i$ ). A parameter is judged to have a significant impact on simulation response through contrasting these two measures with those calculated for the 'dummy' parameter that is known to have no impact.

## Application of SPARTAN to Netlogo Model

This section demonstrates the application of the techniques above to the Netlogo Virus model described previously. In these analyses we treat the model default parameter values are those that create the simulation baseline behavior (*chance-of-recover=50%*, *infectiousness=60%*, *duration=20* weeks), and assign a range of values over which the parameter will be explored (*chance-of-recover=10-90%*, *infectiousness=10-90%*, *duration=5-40* weeks). For technique 1, we set an amount by which the parameter value will be incremented (1%, 1% and 5 weeks respectively). Each simulation was run using the Headless mode of Netlogo, allowing simulations to be run in batches from the command line. For each run, the simulation state is saved at each time-step using the table output functionality included in Netlogo's BehaviorSpace tool. We stress that no additional output function has been added to the model for our purposes, this is produced by Netlogo itself. This ensures the techniques demonstrated here are applicable to the output of any Netlogo model.

## Technique 1: Parameter Robustness

Using the specified parameter space values, SPARTAN generates a Netlogo BehaviourSpace experiment XML file. Netlogo uses this file to perform a sweep of all potential values for that parameter. When complete, SPARTAN can process the simulation response file, taking each parameter in turn and performing a statistical comparison of simulation response when the parameter value is perturbed against behavior at baseline parameter values.

The analysis produces two forms of graphical output, both demonstrated in Figure 1. Figure 1(A) indicates how statistically different each simulation response is for each value assigned to a parameter, in this case the ease at which the virus

spread (*infectiousness*). For there to be no difference, the A-Test result would be 0.5. Large differences occur either side of this, although the direction is not of concern, just the indication of effect. In the case of Figure 1(A), the analysis reveals that a statistically significant alteration is observed for each simulation response with a perturbation of just 1%. Such a result indicates that the simulation is very sensitive to the value of this parameter, and this needs to be assigned carefully.

Figure 1(B) and 1(C) are demonstrations of the result distribution that is also generated for each simulation output measure, for each parameter being examined. In the case of Figure 1(B), this shows how an alteration in the probability of recovery impacts the number of people who die through infection by the virus. This shows the interesting effect that as the chance of recovery initially increases, the number of people who die from the virus also initially increases, up to a point where the number begins to fall. This may not be expected behavior, and may need to be investigated further to determine if there are links between this parameter and the value assigned to others. Such a conclusion can be drawn from global sensitivity analysis techniques that we discuss later in this paper. Figure 1(C) shows how the number of people who die immune to the disease changes as the ease at which the virus spread is increased. This robustness analysis reveals an exponential-like effect, where a further increase in the parameter value does not have much impact on the simulation response. Again this may be a key consideration when setting the value of this parameter.

## Technique 2: Global Sensitivity Analysis using Latin-Hypercube Sampling

Using the latin-hypercube sampling technique, 500 sets of parameter values were generated over the specified parameter space. SPARTAN automatically creates Netlogo experiment XML files containing the chosen parameter values, and from these 500 sets of simulation responses were generated. Each parameter is then analyzed in turn, with output responses sorted by the value assigned to that parameter, and correlations identified as described previously.

Four of the automatically generated analysis plots can be seen in Figure 2. Each plot is for a particular parameter of interest, and a specified simulation response, both specified in the header. The objective is to identify any trends in simulation response between the value of this parameter and the response, although a subset of parameters are being perturbed simultaneously. Figure 2(A) reveals that there is no correlation between the duration of the infection and the number of people who die but are immune. In 2(B) on the other hand, there is a strong correlation between the number of people who die immune to the disease and the probability that they recover, as one would expect, although two other parameters are also being perturbed. This suggests that the researcher should give careful consideration to the value of

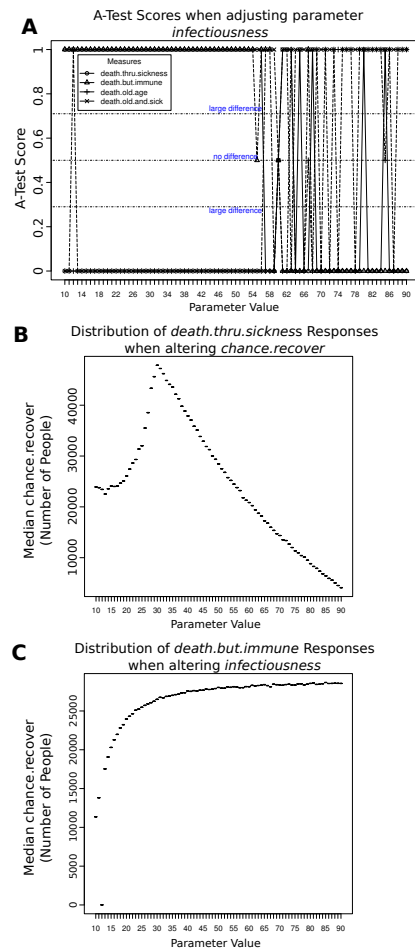


Figure 1: Exemplar robustness analysis output produced by SPARTAN. A: A-Test scores for Netlogo Virus simulation where the ease of catching the infection is perturbed (*infectiousness*). B: Distribution of the number of people who die through the virus when the chance of recovery is perturbed. C: Distribution of the number of people who die immune to the virus when *infectiousness* is perturbed

this parameter. Figures 2(C) and 2(D) are interesting as they reveal correlations between the parameter value and the simulation response for a subset of parameter values. In 2(C), the number of people who die through the infection is correlated with higher values for the chance of recovery, reinforcing the suggestion that this parameter is highly influential. In 2(D), the number of people who die through old age and are currently sick decreases rapidly under low infectious values, with no further trend from around 40% onwards. Such a result can be used to suggest that care is taken with the setting of this parameter, as it may not be influential on simulation response past 40%.

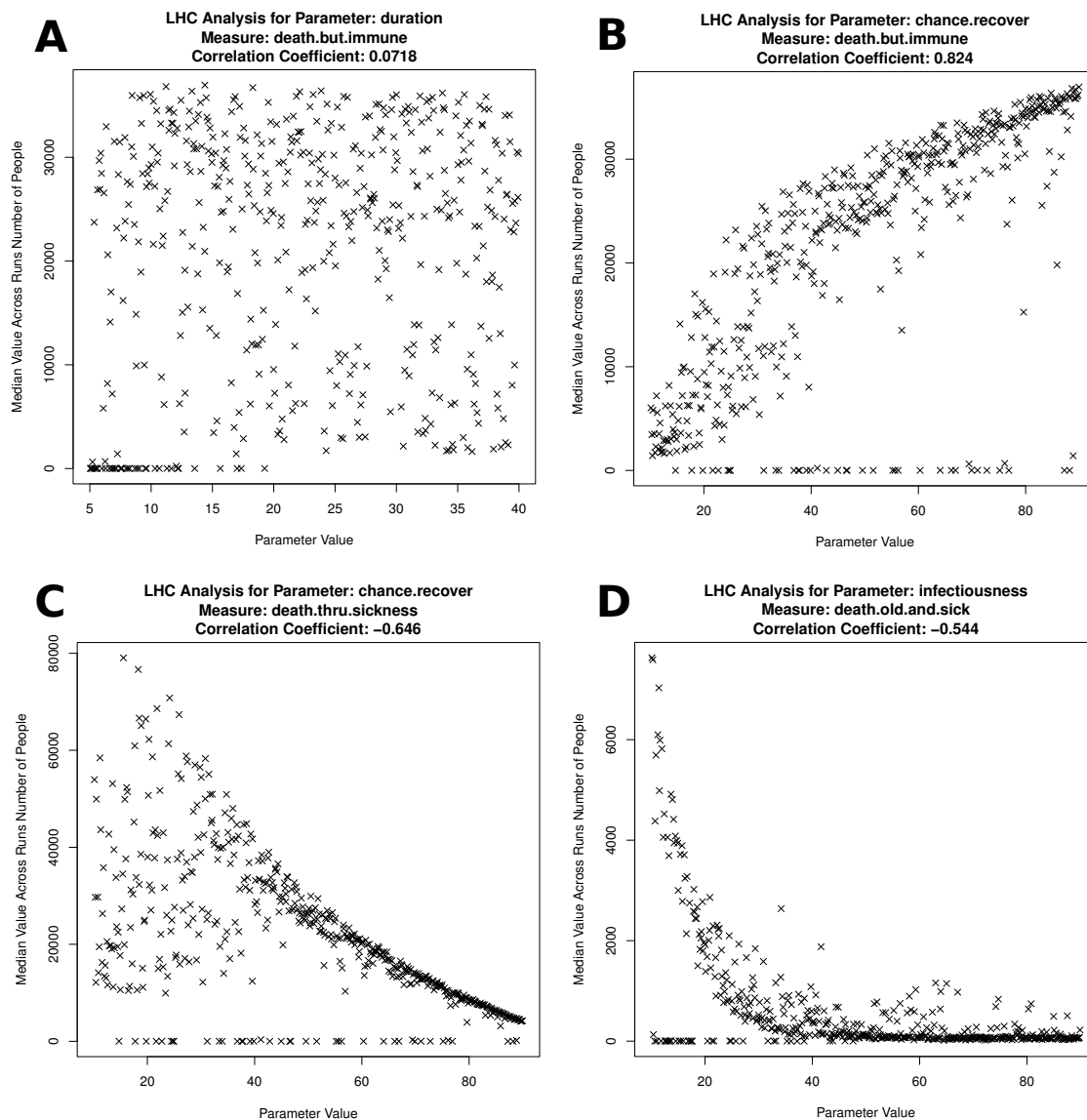


Figure 2: Use of SPARTAN to identify compound effects between parameters, using latin-hypercube parameter sampling. A: Number of people who die immune to the virus, sorted by the value assigned to duration of infection. B: Number of people who die immune to the virus, sorted by the value assigned to the chance they recover. C: Number of people who die through the virus, sorted by the value assigned to the chance they recover. D: Number of people who die through old age while they have the virus, sorted by the value assigned to *infectiousness*

### Technique 3: Global Sensitivity Analysis using Extended Fourier Amplitude Sampling Test

Experiment parameters were generated using the sinusoidal curve sampling method detailed previously. With four parameters of interest (three in the simulation plus the 'dummy'), we have taken 65 parameter values from each frequency curve, and utilized three frequency phase shifts to ensure sufficient coverage of the parameter space, producing 780 parameter value sets. Similarly to Technique 2, SPARTAN automatically produces Netlogo experiment XML files for the chosen parameter values, and from these 780 simulation responses were generated.

The automatically generated graphs for two of the output measures can be seen in Figure 3. As the analysis focuses on each parameter individually, the graph shows the impact that each parameter has on a particular variance measure when that parameter is that of particular interest. The black bars are the  $S_i$  value: the fraction of variance that can be explained by just that parameter when chosen as parameter of interest. The gray bars are the  $ST_i$  value: the fraction of output variance caused by higher-order non-linear affects between this parameter and the complementary parameters. The noticeable result from Figure 3 is that the  $ST_i$  value is high across all parameters for both the shown output measures. This suggests that there is a high degree of dependence between the parameters in this simulation. This is in contrast to our previously published example where this affect was relatively low (Alden et al., 2013). The interesting information in this graph comes from the black bars, the  $S_i$  value. In Figure 3(A), showing the influence of each parameter on the number of people who die but are immune to the virus, the value of the *infectiousness* parameter sensitivity measure is noticeably higher than the other parameters, and the only parameter that is statistically significant in comparison to the 'dummy' measure, known to have no impact on the simulation. This supports earlier analyses that suggest that the *infectiousness* parameter value needs to be carefully considered. A similar conclusion is drawn from Figure 3(B), where again the *infectiousness* parameter is shown to have a statistically significant impact on the number of people who die through virus infection. The chance a person recovers from the infection is also determined to be statistically significant for this simulation response, as one would assume. Interestingly this analysis reveals that the duration of infection has little impact on variance in simulation response.

### Discussion

Although a number of platforms have been developed that aid the development of simulations of complex systems, of which Netlogo is one, similar focus has not been given to the development of statistical tools that analyze the generated results. Platforms are beginning to offer enhanced parameter analysis through filtering and charting, MASS (Multi-Agent Simulation Suite) being one example (Ivanyi et al.,

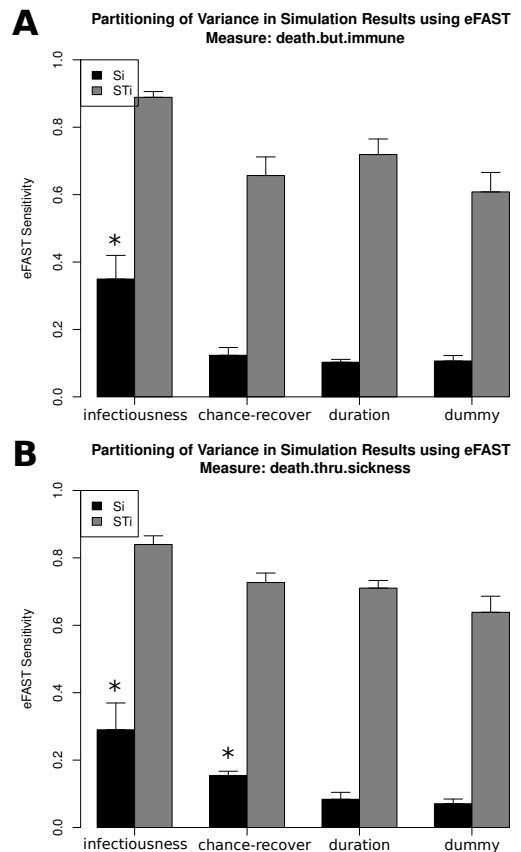


Figure 3: Use of eFAST method within SPARTAN to partition variance in simulation results between parameters. Black Bars:  $S_i$  - the fraction of output variance explained by the value assigned to that parameter when parameter of interest; Gray Bars:  $ST_i$  - the variance caused by higher-order non-linear effects between that parameter and the others explored (includes value of  $S_i$ ). Error bars are standard error over three resample curves. A: Number of people who die immune to the virus. B: Number of people who die due to contracting the virus

2007), yet stress the importance of a link between the platform and a statistical environment (R, MATLAB, etc) for detailed analysis of exported data. Such a statistical analysis is vital for understanding the relationship between the simulation and the real world system it has been built to represent. We developed the SPARTAN package with the objective of providing researchers with the tools to examine this key relationship. Where researchers make the choice to utilize Netlogo as the software platform from which to design their simulation, the BehaviourSpace tool is very useful in providing a means of performing a sweep of potential parameter values. Yet this leaves the researcher to develop their own tools to analyze the simulation responses, to gain an understanding of the behavior of their simulation.

Here we have demonstrated our recent extension to SPARTAN that simplifies the process of performing both local and global sensitivity analyses of a Netlogo model. Through integrating Netlogo and SPARTAN, samples are generated that ensure full coverage of the parameter space, and Netlogo experiment XML files are created automatically. The researcher is now in the position to simply run the batch of experiments from the command line, and analyze the simulation responses using the relevant SPARTAN technique. Statistical information is produced in both graphical and data table forms, easing the identification of any effects generated through parameter perturbation. This provides the researcher with the key information required to gain a full understanding of how their simulation behaves, and where the key parameter pathways lie. To aid the adoption of this approach, we have ensured that SPARTAN is open source and freely available from both the CRAN package repository and our website ([www.ycil.org.uk/software/spartan](http://www.ycil.org.uk/software/spartan)), and provided a detailed tutorial covering each technique. The sample model, data, and command line scripts are also available as exemplars. We see this as a useful addition to the simulation researcher's toolkit.

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### References

- Alden, K., Read, M., Timmis, J., Andrews, P. S., Veiga-Fernandes, H., and Coles, M. C. (2013). Spartan: A Comprehensive Tool for Understanding Uncertainty in Simulations of Biological Systems. *PLoS Computational Biology*, 9(2).
- Alden, K., Timmis, J., Andrews, P. S., Veiga-Fernandes, H., and Coles, M. C. (2012). Pairing experimentation and computational modelling to understand the role of tissue inducer cells in the development of lymphoid organs. *Frontiers in Immunology*, 3:1–20.
- Frank, B. and Baret, P. (2014). Simulating brown trout demogenetics in a river/nursery brook system: The individual-based model DemGenTrout. *Ecological Modelling*, 248:184–202.
- Helton, J. C. (2008). Uncertainty and sensitivity analysis for models of complex systems. In Barth, T. J., Griebel, M., Keyes, D. E., Nieminen, R. M., Roose, D., and Schlick, T., editors, *Computational Methods in Transport: Verification and Validation*, pages 207–228. Springer.
- Ivanyi, M., Bocsi, R., Gulyas, L., Kozma, V., and Legendi, R. (2007). The Multi-Agent Simulation Suite. In *AAAI Fall Symposium Series*, pages 56–63.
- Lee, T., Yao, R., and Coker, P. (2014). An analysis of UK policies for domestic energy reduction using an agent based tool. *Energy Policy*, 66:267–279.
- Luke, S. (2005). MASON: A Multiagent Simulation Environment. *Simulation*, 81(7):517–527.
- Marino, S., Hogue, I. B., Ray, C. J., and Kirschner, D. E. (2008). A methodology for performing global uncertainty and sensitivity analysis in systems biology. *Journal of theoretical biology*, 254(1):178–96.
- Patel, A., Harker, N., Moreira-Santos, L., Ferreira, M., Alden, K., Timmis, J., Foster, K. E., Garefalaki, A., Pachnis, P., Andrews, P. S., Enomoto, H., Milbrandt, J., Pachnis, V., Coles, M. C., Kioussis, D., and Veiga-Fernandes, H. (2012). Differential RET responses orchestrate lymphoid and nervous enteric system development. *Science Signalling*, 5(235).
- Read, M., Andrews, P. S., Timmis, J., and Kumar, V. (2012). Techniques for Grounding Agent-Based Simulations in the Real Domain : a case study in Experimental Autoimmune Encephalomyelitis. *Mathematical and Computer Modelling of Dynamical Systems*, 18(1):67–86.
- Saltelli, A. (2004). *Sensitivity Analysis in practice: A guide to assessing scientific models*. Wiley.
- Saltelli, A. and Bollardo, R. (1998). An alternative way to compute Fourier amplitude sensitivity test ( FAST ). *Comput. Stat. Data Anal.*, 26(4):445–460.
- Saltelli, A., Chan, K., and Scott, E. M. (2000). *Sensitivity Analysis*. Wiley series in probability and statistics Wiley.
- Thiele, J. C., Kurth, W., and Grimm, V. (2012). RNETLOGO: an R package for running and exploring individual-based models implemented in NETLOGO. *Methods in Ecology and Evolution*, 3(3):480–483.
- Vargha, A. and Delaney, H. D. (2000). A critique and improvement of the CL Common Language Effect Size Statistics of McGraw and Wong. *Journal of Educational and Behavioural Statistics*, 25:101–132.
- Wagner, N. and Agrawal, V. (2014). An agent-based simulation system for concert venue crowd evacuation modeling in the presence of a fire disaster. *Expert Systems with Applications*, 41(6):2817–2815.
- Wilensky, U. (1998). *NetLogo Virus model*. Center for Connected Learning and Computer-Based Modeling, Northwestern University. Evanston, IL.
- Wilensky, U. (1999). *NetLogo itself*. Center for Connected Learning and Computer-Based Modeling, Northwestern University. Evanston, IL.
- Yorke, J., Nathanson, N., Pianigiani, G., and Martin, J. (1979). Seasonality and the requirements for perpetuation and eradication of viruses in populations. *Journal of Epidemiology*, 109:103–123.