

Approaches for Resolving the Dilemma between Model Structure Refinement and Parameter Calibration in Agent-Based Simulations

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ABSTRACT

Agent-based simulations form a valuable tool for learning about real world societies and global behaviors of systems emerging from microscopic relationships. Calibration of model parameters for detailed agent-based models is a big problem for standard calibration techniques, due to the large parameter search spaces, long simulation run times, uncertainties in the structural model design and different observation levels upon which the model needs to be calibrated. In this paper we propose several methods to improve the calibration process of agent-based simulations.

Categories and Subject Descriptors

I.6 [Simulation and Modelling]: Model Development, Model Validation and Analysis

General Terms

Experimentation, Algorithms, Measurement

Keywords

Agent-based Simulation, Simulation Calibration

1. INTRODUCTION

Agent-based simulations (ABS) form a valuable tool for studying real world societies and global behaviors of multi-agent systems (MAS) emerging from microscopic relationships. In ABS agents and societies of a real world system are represented explicitly in a simulation model. Autonomous actors are reproduced by agents with their autonomy, individual goals etc. This allows a close mapping between real and modeled system and leads to advantages in relation to macroscopic simulation techniques and also to other micro modeling paradigms like object-oriented simulation, cellular automata or petri networks.

To derive valid results and knowledge from an ABS great

care needs to be put in the model development process. The main problem does not relate to particular specification and implementation languages, but more generally to the (missing) link between macroscopic aggregate behavior and microscopic agent-level model. One major advantage of ABS is that the observation element "individual" equals the modeling element "agent". However it is not clear what properties and behavior, i.e. modeled structure of the real-world agent, actually lead to the measurable aggregate values. This leads to a rather high uncertainty about a valid model structure and consequently about a valid parameter setting. However, parameter calibration can only be done with an appropriate model structure as starting point. On the other hand, whether a model structure is valid can only be assessed with parameter settings. This dilemma is particular to ABS and cannot be addressed by parameter calibration or optimization that take the model and its structure as a black box. Therefore, new methods and techniques have to be developed that combine parameter calibration with model structure refinement for ABS.

2. RELATED WORK

In 1 we described the need for treating parameter calibration and structural refinement of ABS in a combined fashion. As a result the related work is described in three parts:

Black box calibration techniques: In general parameter calibration of simulation models is treated as an optimization problem [4]. The simulation models are adopted as black boxes computing a predefined objective function which measures the overall simulation validity. The problem for direct application of these techniques in ABS is the potentially large level of detail in such simulation models resulting in huge parameter search spaces.

Structural model refinement of ABS: ABM can be designed in a goal-oriented top-down fashion, i.e. starting with an abstract model with the desired macro behavior and adding model detail as required to answer the simulation question, or bottom-up based on the design of local agent relationships. In both cases the step of tuning and refining model structures in case of invalid simulation results is generally handled rather arbitrarily [2].

Systematic Calibration: The calibration issue is not tackled in most agent-oriented engineering methods. Two examples from ABM engineering dealing with calibration are the SADDE methodology [7] which treats the simulation model as a black box employing genetic algorithms (GA) for parameter estimation and the approach described by Calvez

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et al. [1] which also uses black box GA.

3. EXAMPLE MODEL: SHOPSIM

Our application example is an ABS of grocery shopping-behavior in Northern Sweden. In the model stores are defined by their position and seven characterizing attributes like price level, assortment size, quality etc. The shopping agents perceive the store attributes and their individual distance to the stores using some perception functions. They combine the different perceptions into a personal store ranking. Based on this ranking the agents spend their yearly grocery shopping budget. The global objective function of the model measures how precisely the empirical turnovers of the stores are reproduced by the model.

The empirical data for the model validation consists of original statistics of store turnovers and estimations of shopping budgets for the shopping agents. The data used to design and calibrate the target model is fuzzy or simply missing. Many store attributes are based on subjective expert estimations. Further it is unknown which store attributes are actually important for shopping decisions, i.e. whether all or only a subset of the store attributes need to be perceived by the agents. Finally, the potentially over 100,000 agents, evaluating 132 stores each, greatly limits the number of possible parameter configuration evaluations during calibration.

4. MODEL DESIGN AND CALIBRATION

We call our approach a white box calibration approach as opposed to standard black box search (BBS) methods. Our goal is to enhance the efficiency of applied BBS methods by exploiting available expert knowledge and by using calibration methods that explicitly deal with ABM structure.

We suggest a top-down goal oriented analysis of the model and calibration problem. Starting with the conceptual model design, the simulation question(s) to be answered and the necessary level of detail are defined. These form the first two observation levels (macro and micro) upon which we need to ensure model validity. From the simulation question we specify the global objective function for calibration. Based on the analysis of the calibration problem we apply decomposition and abstraction techniques, analyze simplified models and successively refine the model until the desired level of detail has been reached. We do this to overcome arbitrary model changes on local levels.

4.1 Model Abstraction and Decomposition

Based on an analysis of the complexity of the calibration problem one can identify possibilities for increasing the efficiency of applying BBS techniques. The goal is to reduce computational model complexity, to be able to apply individual objective functions for decomposed submodels and to study model relationships on different abstraction levels.

Proposed Proceeding We employ a set of abstraction and decomposition techniques to explore simplified models, create computationally less complex models and analyze local relationships. Abstractions can be aggregations of model units, metamodeling, reductions of heterogeneity or analysis of local interactions. Decompositions can be goal-oriented and on functional, behavioral or temporal levels. A detailed description can be found in Fehler et al.[3].

4.2 Structure and parameter refinement

Several structural model aspects and combinations of these can be responsible for a certain system behavior. We require a technique to efficiently search through possible structural configurations with combined parameter estimation. An example is the calibration of agent perception functions. Agents can potentially perceive several aspects of their environment and act according to reasoning based on these perceptions. However, it may not be known which environmental properties need to be perceived by the agents and if some perception combinations have increased influence on agent behavior. In SHOPSIM we have to identify relevant store attributes and calibrate the associated perception functions.

Proposed Proceeding Our goal is to explore as few perception function subsets (PFS) as possible while identifying the most valid perception model. To search the space of possible PFS we propose to use a combination of a beam search strategy in PFS space, a simulated annealing (SA) search in perception function parameter space and effect analysis using Design of Experiments (DoE) techniques [5]. We start with a subset containing all possible perception functions and optimize its parameters using SA. The next step is to identify the perception functions that are actually responsible for agent behavior. We do this using factorial experiments to determine major and combinational effects up to a preestimated degree using a minimal number of required simulations. Once promising PFS have been determined the experimenter may choose a set of PFS for further investigation following the beam search strategy. The search in structure space may be cut off at any time, if effect analysis suggests no further improvements for certain PFS. Following this procedure in SHOPSIM we explored only 12 instead of potential 127 perception models in order to identify the most valid candidates.

4.3 Validity on multiple observation levels

We want to enforce model validity not only on a global but on several observation levels. Parameter calibration on a single observation level is generally done using objective functions describing degrees of validity on this level.

Proposed Proceeding To ensure model validity on several observation levels we employ behavioral constraints on simulation behaviors during model calibration. Standard constrained parameter optimization uses constraints on the model input parameters, which are tested before and after each parameter configuration evaluation, to guide the search process [6]. We employ behavioral constraints during individual simulation runs. This way we can simply cancel invalid simulation runs, which decreases total calibration time.

4.4 Reasonable introduction of heterogeneity

To keep the parameter search space as small as possible we want to determine small sets of model properties that can be used to describe relevant heterogeneous model aspects, like groups of agents or resources. Additionally we want to determine the error inherent in the available fuzzy empirical data. This is important as we derive information of how good we can actually get during parameter calibration in respect to an objective function comparing simulation output to fuzzy empirical data values.

Proposed Proceeding We explore equivalence classes in model properties to determine relevant heterogeneous model aspects which require additional detail, i.e. parameters. In

SHOPSIM this means that all stores with the same attribute values for a given subset of all possible attributes form a single equivalence class. We seek classes which correctly group stores with similar turnovers. If we measure the deviation of individual store turnovers within valid equivalence classes from the mean class turnover, we can derive information of the calibration error inherent in the fuzzy empirical data. In SHOPSIM we see that for the most appropriate equivalence classes the error inherent in the data leads to a quality of only 60% in global turnover reproduction. This helps us in calibrating the actual model parameters as we now know that we will not be able to reduce the error in turnover reproduction to less than 40% during parameter optimization.

4.5 Reverse engineering approach

Suppose we have a bottom-up designed ABM including expert specified structural aspects and parameters. The simulation results are not satisfying. We need to determine required changes in the simulation model without arbitrary changes in the ABM structure.

Proposed Proceeding We propose to invert the calibration process. Instead of fitting agent model parameters to a given environmental model we reverse engineer an environmental model with properties that fit the predefined agent model. On the one hand the resulting model can be analyzed by the domain expert to identify anomalies and thus required model changes. On the other the reverse engineering approach can be used to abstract certain heterogeneous model relationships allowing faster model calibration.

In SHOPSIM we may have expert designed distance perception functions. The parameters of the remaining perception functions need to be calibrated to complement the heterogeneous distance perception. Here, we abstract the different possible store attributes into a general store "attractiveness" attribute. The idea is to reverse engineer an attractiveness for each store that fits the agents distance perception. Section 4.6 describes an efficient way to do this.

The first gain is that the resulting store attractivenesses can be analyzed for correlation with original store properties. This allows a more directed adaption of model structures and identification of bad empirical data about store attributes. Suppose we want to analyze the micro validity of agent shopping trips based on different bottom up designed distance perception functions. We do this by analyzing them in environmental models theoretically fitted to the agent perception model using reverse engineering. This means we compute what the attractiveness of each store would have to be in order to correctly reproduce store turnovers, if we assume that the local agent model is correct. This allows to focus local behavior validity analysis on the designed distance perception function without having to deal with possible distortions of agent behavior resulting from behavior based on fuzzy data on the non-distance store attributes.

The second gain is that, by reverse engineering, we abstracted the heterogeneous distance attribute of the stores into the store attractiveness attribute which is then perceived homogeneously by the agents. To calibrate the original model, the original non-distance store attributes need to be perceived in such a way that the engineered attractiveness is produced. However, we can now use a simple linear model instead of the computationally expensive ABS to calibrate the parameters of the non-distance perception functions. This allows a much faster evaluation of possible

parameter configurations and thus the application of more exact estimation techniques like gradient based search.

4.6 Calibration of many local parameters

Suppose we want to calibrate numerous local (agent) parameters as in 4.5. The number of parameters exceeds the size that can be sensibly treated using global BBS. We have an estimation of domain expert knowledge how the local environment of an agent influences its parameter values.

Proposed Proceeding We design local update functions which change the agents parameters based on deviation from desired local properties or behaviors. The functions are based on knowledge about local relationships from the domain expert. We update the parameters in an iterative fashion until the values converge. In the SHOPSIM reverse engineering example from the last section we have to calibrate local attractiveness for 132 stores, i.e. 132 parameters, based on a heterogeneous distance agent perception. We defined update functions for each store attractiveness. Depending on the deviation of simulated from the target turnovers the store attractiveness values were adapted. Depending on the chosen perception model 2-5 update iterations were sufficient to calibrate the 132 attractiveness parameters so that the original store turnovers could be perfectly reproduced for given heterogeneous agent distance perception.

5. SUMMARY AND OUTLOOK

In this paper we proposed a framework and associated methods for calibrating ABS designed for prediction and exploration of real world MAS. A main focus was put on the sensible introduction of heterogeneity into the model and the analysis of bottom-up model designs, to overcome the often infeasible trial and error step of parameter and micro level structure refinement. In the future we will further focus on the problem of the introduction of heterogeneity into ABM as this poses a very hard problem to parameter calibration due to the significantly increasing search space size.

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