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Rethinking validation: Efficient search of the space of parameters for an agent-based model

Doina Olaru *, Sharon Purchase

UWA Business School, The University of Western Australia, Crawley, Australia

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ABSTRACT

This paper shows how sensitivity analysis can be used as part of model verification and validation Sensitivity analysis provides insights on where future data validation processes should focus and which inputs may be considered for model reduction. We compared two approaches, one using a systematic variation of parameter values, another using an optimised algorithm to make more efficient the search of their space. Analysis was conducted on an agent-based model that explores the emergence of innovation within business networks, where successful innovation is considered an increase in knowledge and financial resources within the network. The two sensitivity analysis approaches differed both on their time efficiency and on the type of information provided. While the systematic individual sensitivity analysis assisted us in identifying inputs with substantial impact upon the results and suggest solutions for model simplification, the optimised search provided insights on the network resources likely to achieve higher levels of innovation. Genetic algorithms found parameter values that produced different results in the agent-based model.

摘 要

本篇文章描述了如何将敏感度分析用作模型验证和证实的一个部分。敏感度分析指出了未来数据验证流程应该关注的地方，以及哪些数据输入可用作模型降阶。我们比较了两种方法，一种使用系统参数值的变化，另一种使用优化算法以便更有效地搜寻参数空间。我们对在业务网络范围内探索创新出现的基于主体建模展开了分析，成功的创新被视为网络范围内知识和财政资源的增加。两种敏感度分析方法无论在时间效率还是在提供的信息类型方面都各不相同。当中， 系统个体敏感度分析协助我们确定哪些输入对结果带来实质性影响并为模型简化提供解决方案； 而优化搜索则为网络资源如何达到更高层次的创新提供见解。遗传算法确定了某些参数值在基于主体建模中就产生不同的结果。

1. Introduction

Agent-based modelling (ABM) is fast becoming the dominant social simulation paradigm that describes social systems as: complex; highly decentralized; composed of interacting heterogeneous agents; and exhibiting emergent bottom-up behaviour (Bonabeau, 2002; Gilbert and Tierna, 2000; Marks, 2007; Mitleton-Kelly, 2003; Maguire et al., 2006). Agents act with some purpose and their interaction at a micro/individual level – usually through time and space – generates unexpected macro/network level behavioural patterns. These macro level patterns give insight into possible system behaviours that can emerge and are often the focus of the research problem. Yet, before researchers can consider the results of system output behaviour as credible they need to face the challenges of model verification and validation and the lack of common standard procedures on how to conduct them (Louie and Carley, 2008; Marks, 2007; Petty, 2010; Rand and Rust, 2011; Maguire et al., 2006).

Model *verification* is a process that determines whether the programming implementation of the conceptual model is correct, i.e. "is the model made right" (Petty, 2010, p. 332). This process includes debugging the software, testing the logic, looking for incorrect implementation of conceptual models, and verifying calculations (Louie and Carley, 2008; Wang and Lehmann, 2007). Model *validation* answers the question "Was the right model made?" (Petty, 2010, p. 332) and is a process that determines whether the conceptual model is a reasonably accurate representation of the real world and produces outcomes consistent with the

* Corresponding author.
E-mail addresses: donia.olaru@uwa.edu.au (D. Olaru), sharon.purchase@uwa.edu.au (S. Purchase).

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real world (it behaves as expected) (Marks, 2007; Midgley et al., 2007; Rand and Rust, 2011; Windrum et al., 2007). During model validation processes parameters are calibrated/estimated to improve the model alignment with real-world data and ultimately produce evidence that the model is sufficiently accurate for the planned application (accreditation) – Petty (2010). When empirical evidence is lacking, a systematic exploration of different parameters' space provides greater assurance in the validity of the parameter estimates and ranges (Saltelli et al., 2008).

Sensitivity analysis is part of a repertoire of verification (Law and Kelton, 1991) and validation techniques (Richiardi et al., 2006; Petty, 2010; Windrum et al., 2007). Sensitivity analysis is particularly useful as a validation technique for agent based models where it is not clear how the computer code will influence system behavior without running the model (Dancik et al., 2010; Bianchi et al., 2007). There are different approaches when considering sensitivity analysis: global sensitivity analysis where a sensitivity index is calculated; sensitivity analysis on individual parameters (Confalonieri et al., 2010; Perz et al., 2013; Ligmann-Zielinska, 2013) and optimised sensitivity analysis that focuses on optimising an objective function (Stonedahl and Wilenski, 2011). Global sensitivity analysis considers the model holistically, while individual sensitivity analysis considers how individual parameters impact model output. Windrum et al. (2007) highlight that sensitivity analysis should also be used to explore the validity of initial conditions and assumptions, the relationship between micro and macro parameters, and timing of mechanisms within the code.

This paper reports on different techniques to sensitivity analyses (*BehaviorSpace* and *BehaviorSearch*) performed using global, individual (traditional) and an objective function guided search (optimization) sensitivity analysis. The paper contributes to the literature on validation of social simulation by comparing these different sensitivity analysis techniques and discussing the benefits and disadvantages of each technique. Overall, this paper aims at exploring different sensitivity analysis processes that will allow researchers to improve the efficiency of their validation procedures.

2. Model description

A complexity perspective is useful when considering innovation networks (Dougherty and Dunne, 2011; Andriani, 2011) and aligns well to the social reality of the real-world system (Byrne, 2012). Innovation occurs when agents within business networks interact to successfully develop new ideas. Multiple agents with resources interact to generate innovations, consequently leveraging the creation of innovations developed externally (Gilbert et al., 2001). This perspective considers the *business network* as the medium for generating innovations, in other words, innovation is a collective endeavour in which networked agents work together to innovate and bridge the gaps between resources and applications (Hoholm and Olsen, 2012; Dougherty and Dunne, 2011).

Our model includes three types of agents: financial backers representing partners who invest in new ideas; manufacturers representing organisations that commercialise innovations; and R&D companies representing science partners from which innovative ideas emerge (Ferrary and Granovetter, 2009; Powell et al., 2005). The model also includes parameters considered important within the literature: network configuration (Powell et al., 2005; Hoholm and Olsen, 2012; Ferrary and Granovetter, 2009); social capital (Carmona-Lavado et al., 2009; Partanen et al., 2008) and complementary technologies (Andriani, 2011; Dougherty and Dunne, 2011).

The ABM model was initially built in NetLogo 4.0 and further refined in version 5.0.4. In the network, the interaction between agents is stochastic and the agents have the choice to connect to a number of other agents they "prefer". Social capital (links) tunes the degree of interaction between agents – reflecting the agent's ability to access network resources – is mimicked in the network via the strength of links. Agents have various endowments (deterministic and stochastic elementary properties) such as type, financial and knowledge resources, or uniqueness of knowledge. After specifying the behavioural rules for agents and their interaction, we explored the consequences at a network level. Detailed description of the model inputs can be found in Purchase et al. (2008) and Denize et al. (2012). The macro variables containing the information relevant to the analysis of the system are averages of financial ($\overline{F_{fi}}$) and knowledge resources ($\overline{K_{fi}}$) and change in the total resources (Δ):

$$\Delta = \frac{\sum_i [\gamma(\beta K_{oi}^{\alpha}) + (1-\gamma)\delta F_{oi}]}{\gamma K_{oi} + (1-\gamma) F_{oi}}, \tag{1}$$

where γ is the weight combining the financial and knowledge resources, and α, β and δ are parameters that model the increase or decrease of resources, moderated through social capital (Table 1). α and γ model the increase or decline of knowledge resources using a power function (specialised, in-depth knowledge increases much more than general knowledge). Table 1 lists the input parameters used in the model and subsequent sensitivity analysis.

The complex relationships governing the knowledge transformations can be summarized as follows:

$$\alpha = \begin{cases} >1 \text{ if knowledge uniqueness} \geqslant \Theta \\ 1 \text{ if knowledge uniqueness} < \Theta \text{ and medium} - \text{high social capital} \\ <1 \text{ if knowledge uniqueness} < \Theta \text{ and low social capital} \end{cases} \tag{2 a}$$

$$\beta = \begin{cases} >1 \text{ if knowledge uniqueness } \geqslant \Theta \cap \text{ high social capital} \\ 1 \text{ otherwise} \end{cases} \tag{2 b}$$

F_{oi} and K_{oi} represent the resources hold initially by the agents. This amount depends on the profile and size of each type of actor, with FB, for example expected to present a higher level of financial resources, and R&D, a greater level of knowledge resources. As a result of the interaction (re-combining resources, and social capital,), these resources are multiplied or depleted (F_{fi} and K_{fi}) and converted into innovation, such that at the end of a given number of iterations (n), the network "produces" new knowledge.

Sensitivity analysis is conducted with all input variables (see Table 1) for three output/objective functions (change in knowledge resources; change in total resources, and relative change in network resources). Table 1 provides the ranges of input parameters "tested" in the sensitivity analysis.

3. Sensitivity analysis

This paper uses global, individual/traditional and optimisation sensitivity analyses as important components of our validation procedures to improve model credibility. Benefits of conducting global sensitivity analysis include: ease of communication of results to non-technical managers; ability to incorporate more than one input variable within the sensitivity analysis (called interactions); ability to incorporate non-linearity within the model; and ability to include feedback loops within the sensitivity analysis (Perz et al., 2013; Ligmann-Zielinska, 2013). Yet, relying *solely* on a global sensitivity index is not recommended,