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# Using docking/replication to verify and validate computational models

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Conventional practice in modelling requires checking that a model is correct with respect to its conceptualisation (verification) and that it corresponds to the real world phenomenon modelled (validation). Verification and validation assure the external and operational validity of a model (its quality). In settings where data for estimation is not readily available, the behaviour of the computational model and its results are questionable. An alternative approach that has been recently gaining attention is docking or replication, which is a process where one model is tested against another to see if they produce the same results.

This paper reports on the docking experience and validation stages performed when replicating a fuzzy logic (FL) model's findings with an agent-based model (ABM) in the context of innovation in business networks. Using two modelling paradigms and software programs, we modelled in an 18 month-interval a network of three agent categories, which collaborate on adopting and advancing new ideas and technologies. The network links describe relations between agents, which drive processes of innovation. The autonomous agents are organisations of different sizes, characteristics, and roles and they interact/share resources/collaborate for the purpose of adoption and diffusion of innovation that fits with the organisation's goals. Depending on their resources, there is scope for innovation or otherwise. In addition, the environment can foster or hinder the innovation processes.

The verification and validation of these two models involved several stages:
1) Expert judgement - the structure of the conceptual model is supported by literature and discussions with colleagues in various forums;
2) Checking the correspondence between what is emerging from the model and what is expected to be seen in the real world (passing the believability test); it is desirable for the model components to adequately represent a real equivalent behavioural effect but as real data was not available at the time of designing the models, the alignment of the model results to expectations acts as an external validation of the model;
3) Internal validity – assessing consistency by changing input data distributions and analysing extreme conditions.
4) Docking (also known as alignment or replication with contrasting alternative theories) - comparing the results of the two different modelling approaches. The models ensured the distributional equivalence, but they were not identical.

As both models used the same parameters, we believe that the differences in results arose only from relaxing the restrictive assumptions in the FL or ABM models. The ABM results matched the FL conditions tested. The stochastic ABM generated a distribution of outcomes caused by random encounters among agents, while FL generated an ensemble of crisp values as result of multiple rules of interaction applying simultaneously. The replication experience has been a positive one. Although this does not justify the models' acceptance, the docking results encourage us to pursue collecting data to validate empirically both models in the near future.

We conclude with some thoughts from Kleindorfer et al. (1998) in relation to various positions in the philosophy of science with respect to validation: in the simulation literature there is a continuum of opinions ranging from extreme objectivist (model validation can be separated from model builder and its context) to relativist ("model and model builder are inseparable" and "validity is a matter of opinion" – Kleindorfer et al., 1998:1097). Their debate leads to a perspective that simulation modelling should not follow a prescriptive set of approaches to validation, but rather modellers should "responsibly and professionally argue for the warrant of the model".

***Keywords:*** *docking, replication, validation, simulation*

## 1. INTRODUCTION

Development of modelling techniques and their large adoption as commonly accepted research instruments/standard methods depends on their accuracy and transparency (Richiardi et al., 2006; Midgley et al., 2007; Wang and Lehman, 2007), which in turn calls for standards of evaluation in modelling. Hence, for new approaches/techniques to become mainstream research approaches and realise their scientific potential, further work needs to be conducted into how models are validated and verified (Cioffi-Revilla, 2002; Maguire et al., 2006; Richiardi et al., 2006).

A number of researchers recently highlighted the need to develop a suite of "best practices" allowing them to validate and verify the computational simulation models they develop (Maguire et al., 2006; Wilensky and Rand, 2007; Richiardi et al., 2006; Louie and Carley, 2008; Wang and Lehman, 2007; Windrum et al., 2007). Verification (checking that a model is correct with respect to its conceptualisation) and validation (checking that a model corresponds to and explains the real world phenomenon modelled) support the external and operational validity of a model but if data for estimation is not readily available, the behaviour of the computational model and its results are questionable (Wilensky and Rand, 2007). Proof that a simulation model is correct is in general difficult especially if traditional validation methods are not applicable (Wilensky and Rand, 2007; Louie and Carley, 2008). Statistical validation should not be seen as providing the “absolute” validity of the model (Robinson, 2005; Midgley et al., 2007) and alternative approaches need to be considered. *Docking*, *alignment* or *replication* of the models is such an alternative approach that has been recently gaining increasing attention. Docking is a process where one model is tested against another to see if they produce the same results (Maguire et al., 2006). If different implementations of a conceptual model produce similar findings, that lends support to the models in mimicking the real world phenomenon. This paper briefly reviews literature focusing on the lack of standards for validation and reports on the docking experience and validation stages performed when replicating a fuzzy logic (FL) model’s findings with an agent based model (ABM) in the context of innovation in business networks (Purchase et al., 2008). Replication standard holds that sufficient information exists to understand, evaluate, and build upon a prior work, so that results can be replicated without any additional information. In our case, the same researchers built the two models for exploring innovation creation and change of resources in business networks within 18 months, making the replication effort less arduous.

## 2. APPROACHES TO VALIDATION AND VERIFICATION

Validation has been defined as “substantiation that a computer model, within its domain of applicability, possesses a satisfactory range of accuracy consistent with the intended application of the model” (Kneppel and Aragno, 1993:3 cited in Klein and Herskovitz, 2005: 305). Traditionally, this requires empirical evidence to check/compare the output of the model. If this does not pass the scrutiny or the test cannot be performed, the model cannot be demonstrated as correct. Many researchers have recently addressed the verification and validation standards and suggested other avenues or provided frameworks for validating simulation models - Klein and Herskovitz (2005), Richiardi et al. (2006). Klein and Herskovitz (2005) examined the contrasting philosophies of science of Popper, Quine, and early-period Putnam and recommended Popper’s framework for validating models. According to Popper’s falsificationism, models should be submitted to severe tests and if a model “passes such test by remaining not falsified, it is viewed as only a conjecture that will do for now, a mere tentative representation of reality” – Klein and Herskovitz (2005): 307. With this stance, statistical hypothesis testing is labeled as falsificationist and the impossibility to support consistency between model results and real data is translated in rejection of the model. Models may be temporarily validated and they need to be continuously reassessed. Quine shares Popper’s view that a theory can never be proven true, but unlike Popper, Quine held that “neither can it be proven false” (Klein and Herskovitz, 2005: 313). In the early-period Putnam’s perspective, a “scientific theory‘s long term record of making correct predictions is grounds enough for accepting the theory as at least approximately true” - Klein and Herskovitz (2005): 316. Accordingly, “there can be no definitive rejection of a model, and so there are no incentives for model improvement” (p. 318).

Richiardi et al. (2006) highlighted the need for a common protocol for validating and reporting simulation models. Their review includes five types of validity for simulation models that are theory and data based: *theory validity* (validity of theory relative to real-world system); *model validity* (model relative to theory); *program validity* (program relative to model); *operational validity* (theoretical concepts relative to their indicators); and *empirical validity*. Drawing on Sterman (1984), Richiardi et al. (2006) also suggest heuristic questions to address different validity facets: structure verification; extreme condition and boundary adequacy for validity of model structure or behaviour reproduction, anomalies, family member, extreme policy for validity of model behaviour (Richiardi et al., 2006:8). Within their framework a number of different techniques can be used for validation, with some techniques covering more than one category of model validation. Similar views are found in many other papers addressing modeling validity. Louie and Carley (2008) distinguish between *validation processes* (series of steps for validation) and *techniques* (individual methods applied to ascertain the validity of the model - or a part of it) and advocate that the validation process should be linked to the purpose and context for which the model is being developed (p. 243). They also differentiated among three types of validation: conceptual, data, and operational validity, each conferring a different type of credibility to a model. The *conceptual validity* refers to the extent to which model theory and assumptions are appropriate for the model. *Validity of data* ensures that data is appropriate, accurate, sufficient for the model, whilst the *operational validity* looks at the extent to which the model output matches the real system for the purpose it was built.

This preamble on validation issues stresses two important aspects: i) there is no consensus among researchers on what is considered validity and how to address it and ii) there are degrees of validity (relativity in judging validity) that can be achieved using a combination of instruments/methods.

Although validation against real data is desired, lack of available experimental observations compelled us to search for alternative ways to assess the predictive capabilities of our models. Our choice was ***docking*** (Axtell et al., 1996; Wilenski and Rand, 2007). Axtell et al. (1996) developed the basic concepts and methods of docking to explore how alignment of the results of one computation simulation with the results of a replicated model can assist model validation. Model-to-model replication differs from model re-implementation (re-writing code) and docking only refers to model replication (the model being re-written with different mechanisms or processes used to conduct the simulation). Docking/replication assures the researcher that the model outcomes are stable (repeatedly generated) and not produced by exceptional circumstances (Wikensky and Rand, 2007) and thus it allows the researcher to establish an indirect relationship between the theoretical underpinnings of the model and its results. Replicated models differ across six dimensions: time; hardware; languages; toolkits; algorithms and authors (Wilensky and Rand, 2007), with the different mechanisms being the most important aspects of replication (Axtell et al., 1996).

However, replication alone is not sufficient for validation. Criteria are required to delineate the extent of replication achieved and the equivalence of the results. Axtell et al. (1996) provided three categories for assessing docking: *numerical identity*, *distributional equivalence*, and *relational alignment*. Numerical identity suggests results that are numerically the same in the two models. Distributional equivalence considers that the distributions of results are statically indistinguishable. Relational alignment highlights that the patterns of interactions in the models as the same across the two models (Axtell, 1996).

Other techniques that can be applied for validation and verification but are not addressed here include: developing simulation rules or indicating that patterns of model results are consistent with real-world processes through methods such as case analysis; discourse analysis and action research (Richiardi et al., 2006; Maguire et al., 2006).

## 3. MODELLING INSTRUMENTS

### 3.1. Model design/structure

Our purpose is to model changes in the information/knowledge and financial flows within a business network with actors interested in innovation. This is a symbolic network (Watts, 2004) where links describe abstract relations between agents collaborating for sharing new ideas and advancing technologies and the model identifies what drives processes of innovation (Figure 1). The dynamics of innovation involve important characteristics of complex systems[1] (agent heterogeneity, non-linear interactions, network effects, stochastic elements and uncertainties), which led us to choosing as appropriate modelling approaches agent-based modeling (ABM) and fuzzy logic (FL)[2].

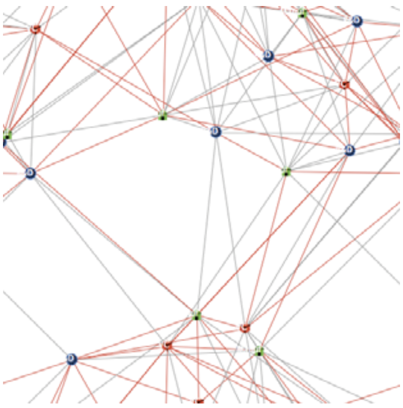

**Figure 1.** Network structure

[1] Complexity is used here in the technical sense that the “behaviour of the system as a whole cannot be determined by partitioning it and understanding the behaviour of the parts separately, which is the classic strategy of the reductionist physical sciences” – Gilbert (2004):3.

[2] The ABM model was built in NetLogo 4.0 and the FL model in CubiCalc 2.0.

The model includes three types of actors with relevant roles in the innovation network (venture capitalists VC, manufacturers M, and R&D companies); these organisations have different sizes, characteristics, and roles; they interact/share resources/collaborate for adoption and diffusion of new ideas that fit with the organisations' goals. Hundred actors are randomly generated in the network then fully connected. The ties can be strong or weak (depending on how long the agents have been in contact to each other, the mutual services and amount of joined activities they have) and through them money and information flow; spreading of the agents tends to reduce the intensity of the interactions via a gravity function moderating the links parameters. Depending on the resources they can put together, there is scope for innovation or otherwise; R&D activities require monetary resources and reduce the capital stock of the VCs or manufacturers, but the capital will be refreshed by successfully introducing a further innovation (considerable increase in the knowledge and skills).
Environment conditions can foster or hinder the innovation.
The agents have local, micro-knowledge and do not know what happens within other relations; the collaboration does not involve selective search for potential partners, interaction being a stochastic element.
After specifying the behavioural rules for agents and for their interaction, we explored the consequences at the level of the network within the models. Macro-variables such as: financial (F) and knowledge (K) resources, and change in the total resources (I) were compared across agents. The model evolves in discrete steps and at the end of one run, the actors can assess their resources and position in the network.

### 3.2. Agent-based modeling (ABM)

Agent-based modelling is an alternative to classical thinking where systems' evolution is expressed using functions, equations, and algorithms. ABMs operate with agents, environment, objects which interact with each other. In addition to providing a natural and intuitive description of a complex system, ABMs capture emergent behaviour (Bonabeau, 2002; Watts, 2004): ABMs "show how simple and predictable local interactions can generate familiar but enigmatic global patterns, such as the diffusion of information, emergence of norms, coordination of conventions, or participation to collective action." – Macy and Willer (2002: 143). This means entities endowed with certain behaviours and interactions lead to complex spontaneous dynamics in the system and large changes could be driven by even subtle modifications maybe imperceptible to actors having only local knowledge of the network (Windrum et al., 2007).

The widespread use of ABM in many fields is a response to the complexity of the real world phenomena and data availability and increased computational advances have facilitated it (Pyka and Fagiolo, 2005; Louie and Carley, 2008).

Fundamental characteristics of the ABM regard (Macy and Willer, 2002; Windrum et al., 2007):
- Autonomy of agents – agents make independent decisions and the system is not directly modelled as a globally integrated entity, but self-organising patterns dictate the behaviour of the whole;
- Interdependence of agents – direct and via environment, network; the collective action result depends on the structure of the network (Watts, 2004) and the emergent structure is not the magnification of single agent behaviour at a larger scale (Gilbert, 2004; Windrum et al., 2007);
- Simple rules – global complexity does not necessarily reflect the cognitive complexity of individuals; ABM explore the simplest set of behavioural assumptions required to generate a macro pattern of interest (Bonabeau, 2002);
- Adaptive/flexible behaviour – "agents adapt by moving, imitating, replicating, or learning, but not by calculating the most efficient action" (Holland, 1995:43, cited in Macy and Willer, 2002:146); agents use heuristics, adaptation, 'evolution'/learning to change their strategies;
- Dynamics nature – always in motion (Bonabeau, 2002; Gilbert, 2004); the state of the system is path dependent and by definition out-of-equilibrium (Pyka and Fagiolo, 2005; Windrum et al., 2007).

### 3.3. Fuzzy logic (FL)

The second modelling approach provides an ideal framework to deal with independent layers of data of varying degrees of uncertainty/confidence, 'imprecision', membership. FL is another paradigm departing from traditional mathematical approaches and opening the door to a new way of defining knowledge using statements that can be true to a certain degree. Born to deal with degrees of truth (instead of the binary Boolean logic), tolerant to 'ambiguous', noisy data, and operating with linguistic expressions for reasoning, FL started to spread in numerous domains in the last decades (Cordón et al., 2001). The mathematical set theory and logic are augmented in FL by making fundamental changes to the ideas of set membership and to the logical operations.

The motivation for FL is provided by the need to represent propositions such as: "Companies X and Y are close friends.", "Most R&D do not have very high financial resources.", "Current market conditions are not favourable.", or "This information is not relevant at all."

While traditional set theory defines membership as being either being true or not, FL allows us to address growth in a comprehensive manner including the fuzziness about what the agent or innovation really is, the fuzziness of antecedents of innovation, and the interactions between agents.
The reasoning system is based on techniques that combine those membership functions using IF-THEN rules of behaviour. There are several structures of the fuzzy systems (including fuzzification interface, inference engine, knowledge base, defuzzification), but in this research we used the Mamdani fuzzy rule based system (Cordón et al, 2001).

Each rule has a number of inputs/antecedents and one output/result. The knowledge base for our FL model includes 486 "IF-THEN" rules expressing the expert field knowledge of the authors. Multiple rules fire at the same time and they may have various weights.

The FL model is not a micro-scale model, and the results are reflecting the behaviour of the clusters of agents.

## 4. VALIDATION PROCESS AND TECHNIQUES

### 4.1. Overview

In this research we addressed the conceptual validity, and partly the validity of data and operational validity described by Louie and Carley (2008). The *conceptual validity* was assessed via experts, *data* via sensitivity to parameter changes, and *operational* via docking/replication (Figure 2). The two dotted lines indicate techniques for operational validity not possible in our case with the usual empirical analysis. Replication (comparison of two models developed in alternative paradigms) instead supports the validity.

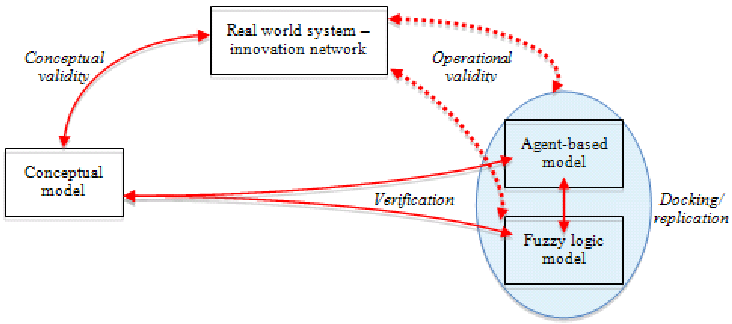


**Figure 2.** Model validation (Adapted after Loiue and Carley, 2008: 244).

### 4.2. Validation approaches and stages

In the innovation network models, the validation involved several stages, presented in Table 1. The left column presents types of validation and the right column how the validation was performed and its results.

**Table 1.** Validation approaches and stages

| | |
|---|---|
| *Conceptual validity* – based on theories | Structure of the model is supported by literature (Denize et al., 2007) |
| *Expert judgment* – discussions with colleagues in various forums (seminars, conferences); as indicated Bonabeau (2002), validation of ABM of social processes inevitably assumes a degree of arbitrariness and subjective/expert judgment | On numerous occasions (IMP and ANZMAC conferences) we found confirmation for the representation of each dimension in the model and for the hypotheses included |
| *Input validation* – ensuring that the fundamental conditions incorporated in the model reproduce aspects of the real system | Ex ante - verification of the ranges of the parameters of the models (decay of irrelevant information, relativity between financial and knowledge resources for the three classes of actors) |
| *Believability test* - checking the correspondence between what is emerging from the model and what is expected to be seen in the real world; although not sufficient for concluding that the models are correct, indication that model components adequately represent a real equivalent behavioural effect is necessary when real data is not available | Examples of judging the model output include:<br>- a) effect of network density<br>Network density creates clusters with enhanced ability to innovate, showing/confirming that geography is important; we emphasise the model does not generate a particular pattern of clusters, but the grouping that emerges displays the same "signature" – greater resources and innovation creation.<br>- b) effect of network size<br>The smaller the network, the greater the probability for an actor to interact with a previous actor.<br>- c) analysis of extreme conditions – reducing to zero the resources for each type of actor<br>The network collapses according to the rules. |
| *Internal validity*<br>– comparing the results from simulations with various random seeds for assessing consistency<br>- changing the type of the noise | Statistical tests confirmed repeatability (no statistical difference between runs)<br>The type of noise was explored by comparing results from:<br>- a) changing the normal distributions to uniform distributions and<br>- b) changing the parameters of the normal distributions<br>Normal distribution of effects was obtained in all situations (K-S test) |

| | |
|---|---|
| *Sensitivity analysis* – what-if scenarios to ascertain the effect of inputs upon the model's output; we conducted sensitivity with respect to: strength of relationships and proportion of actors | Sensitivity analysis revealed important effects and we invest to collect data in those fields. The hypotheses that guided the experimental design (behavioural space) were:<br>- stronger ties between agents are associated with generation of new ideas and adoption of innovation if the relevant knowledge flows between R&D to users of innovation;<br>- knowledge is "lost" if there is no good soil to seed it (at least moderate strength of interactions and resources to develop/implement the innovation);<br>- imbalanced number/proportion of the three types of agents may hinder the realisation of new ideas; when extreme condition tested – type of actor missing – this led to disfunctionalities in the network. |
| *Docking* – comparing the results of the two different modelling approaches (Axtell et al., 1996; Wilensky and Rand, 2007; Purchase et al., 2008). | Over 1,000 runs for the FL model and over 5,000 runs for ABM<br>The models ensured distributional equivalence, but they were not identical, as it is impossible to get numerical identity given the two distinctly different simulation mechanisms used. Both models used the same parameters, so we believe that the differences in results arose only from relaxing the restrictive assumptions in the FL or ABM models. Fuzziness was not possible in the ABM, while emergence and extended time periods were not possible in the fuzzy logic model. The stochastic ABM generated a distribution of outcomes caused by random encounters among agents, while FL generated an ensemble of crisp values as result of multiple rules of interaction applied simultaneously.<br>Both simulation models produced three clusters: steady, awesome (increased resources I > 0), and vulnerable (declined resources I < 0) (Figure 3). Cluster profiles were similar in the two data sets (Figure 4). The statistical results indicate a high level of equivalence. |

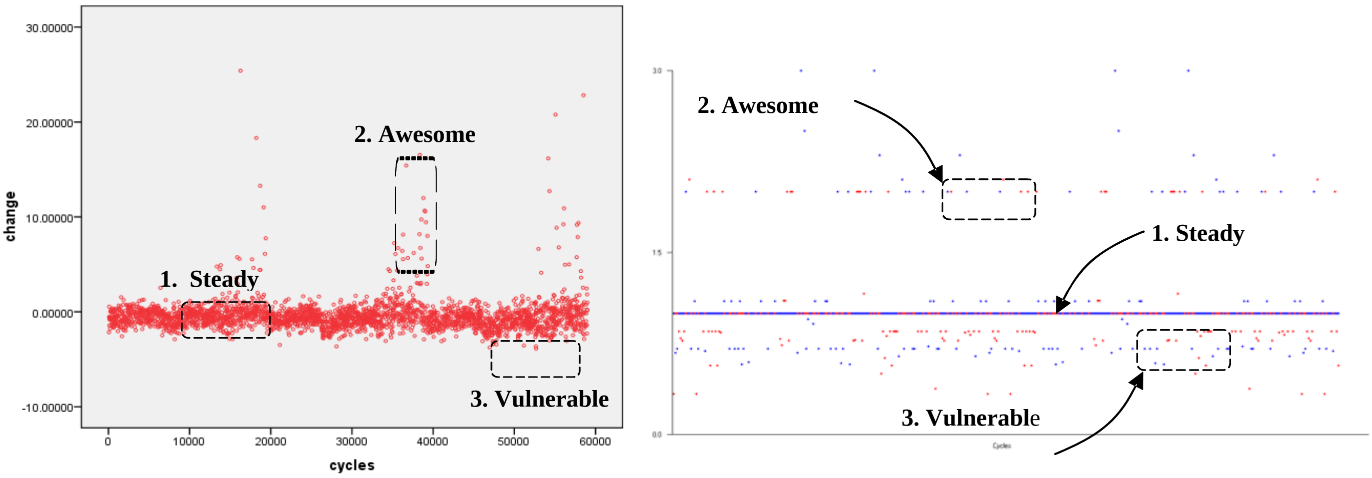


**Figure 3.** Clusters of agents based on their resources

The "awesome" cluster includes actors with higher level of relevant knowledge resources, with stronger ties/collaborations with other actors, thus a more privileged position in the network. The "vulnerable" cluster comprises actors with low level of knowledge resources and weak ties, whereas the "steady" cluster has a mix structure in both models.

MANOVA analysis was performed to compare the clusters and we found that clusters were associated with statistically different measures of resources, relations, and change (multivariate and between subject tests p<0.001), but the type of model did not have a statistically significant effect on the results (p=0.069).

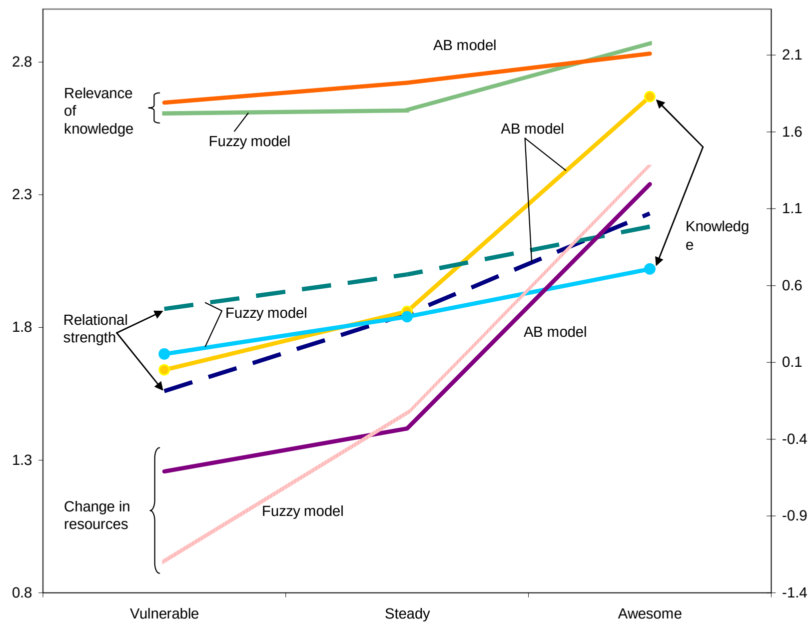


**Figure 4.** Profile of clusters of agents in the two models

## 5. CONCLUSIONS

Our docking exercise sheds light on the relations driving innovation in business networks and generates synthetic data under a variety of conditions to represent possible situations in the real world innovation networks. This is because ABM and FL models enable more realistic representations of complex dynamic systems. The models explore the relationships between agent behaviour and the emergent behaviour of the innovation network using flexible structures. In the same spirit as most ABM applications, we were more concerned with the theoretical development and explanation of phenomena than with prediction, therefore the lack of real data was not considered a hurdle for developing the models. FL and ABM models were incrementally and transparently developed, with ad-hoc adjustments arisen from theoretical base and discussions with peers, in order to arrive at a better representation of the innovation network, to understand the factors and assumptions. The models produced similar results. However, one successful cross-validation does not justify the model acceptance and we will further improve the models, especially considering some inherent docking difficulties: the ambiguity and uncertainty built into the FL model was not possible in the ABM. The experimental generation of values in the FL used linguistic variables (low, medium and high) with membership functions, while the ABM required probability distributions for each of the variables. Another difficulty is that the FL model only gave results at the network level while the ABM at the individual level.

Through replication, we gained confidence in the algorithms and implementation and the results are plausible. Within their domain of applicability, the models have a satisfactory range of accuracy and support our hypotheses on innovation creation and the stance that the empirical validation should not be the primary basis for accepting or rejecting a model.

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